

1 The Bose-Hubbard Model

The Bose-Hubbard (BH) model describes the ground state of spinless itinerant bosons on a 1D lattice, subject to periodic boundary conditions, and on-site particle interactions. The Hamiltonian matrix representing the BH model is:

$$H = - \sum_{i,j} t_{i,j} b_i^\dagger b_j + \frac{U}{2} \sum_i n_i(n_i - 1) - \sum_i \mu_i n_i \quad (1)$$

where $t_{i,j}$ is the hopping amplitude between sites i and j , U is the on-site interaction strength, μ_i is an on-site chemical potentials, b_i^\dagger (b_i) creates (annihilates) a boson on site i , and n_i counts the number of bosons on site i .

In the Fock configuration basis, the interaction potential and the chemical potential terms are diagonal operators, while the first term, the kinetic energy operator, is not. The Hamiltonian can be rewritten as:

$$H = H_1 + H_0 \quad (2)$$

where $H_1 = - \sum_{i,j} t_{i,j} b_i^\dagger b_j$ is the off-diagonal term, while $H_0 = \frac{U}{2} \sum_i n_i(n_i - 1) - \sum_i \mu_i n_i$ is the diagonal term.

The matrix elements of the diagonal and the off-diagonal parts of the Hamiltonian can be explicitly determined by sandwiching the operators between basis states. Matrix elements of each of these operators will show up as factors of the partition function. In the next section, explicit expressions for these elements will be derived.

1.1 Matrix elements

In this section, the matrix elements of the diagonal and off-diagonal parts of the Bose-Hubbard Hamiltonian will be derived. Additionally, we will introduce a so-called "worm operator". This off-diagonal operator is not traditionally part of the Bose-Hubbard model. Nevertheless, for convenience when implementing the Worm Algorithm, the Hamiltonian will

include this term. Thus, matrix elements of the worm operator will also show up as factors of the partition function and will be derived in this section.

1.1.1 Potential energy and chemical potential

Due to H_0 being a diagonal operator and the basis states being orthonormal, the diagonal matrix elements are rather simply obtained:

$$\langle \alpha' | H_0 | \alpha \rangle = \langle \alpha' | \epsilon_\alpha | \alpha \rangle = \epsilon_\alpha \langle \alpha' | \alpha \rangle = \epsilon_\alpha \delta_{\alpha', \alpha} \quad (3)$$

where ϵ_α is the off-diagonal energy of Fock configuration α , and $\delta_{\alpha', \alpha}$ is a Kronecker-Delta function. In other words, the matrix elements vanish when the configurations α' and α are different, and become ϵ_α otherwise.

1.1.2 Kinetic energy

The off-diagonal elements of the Hamiltonian are given by:

$$\langle \alpha' | H_1 | \alpha \rangle = - \sum_{i,j} \langle \alpha' | t_{i,j} b_i^\dagger b_j | \alpha \rangle \equiv H_1^{\alpha', \alpha} \quad (4)$$

Recall the definition of the bosonic creation and annihilation operators:

$$b^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle \quad (5)$$

$$b |n\rangle = \sqrt{n} |n-1\rangle \quad (6)$$

The basis states can be expressed as:

$$|\alpha\rangle = |n_1^\alpha, n_2^\alpha \dots, n_L^\alpha\rangle \quad (7)$$

where $n_i^\alpha = b_i^\dagger b_i$ is the number of particles on site i of the configuration $|\alpha\rangle$, and L is the number of lattice sites. In this representation, acting first with the annihilation operator on site j , then acting with the creation operator on site i produces the following result:

$$b_i^\dagger b_j |n_1^\alpha, n_2^\alpha, \dots, n_L^\alpha\rangle = \sqrt{n_j^\alpha(n_j^\alpha + 1)} |\dots, n_j^\alpha - 1, \dots, n_i^\alpha + 1, \dots\rangle \quad (8)$$

Only sites i and j are modified. The matrix element in Eq. (4) becomes:

$$H_1^{\alpha,\alpha} = - \sum_{i,j} t_{i,j} \sqrt{n_j^\alpha(n_j^\alpha + 1)} \langle n_1^{\alpha'}, n_2^{\alpha'}, \dots, n_L^{\alpha'} | \dots, n_j^\alpha - 1, \dots, n_i^\alpha + 1, \dots \rangle \quad (9)$$

Due to orthonormality of the basis states:

$$\langle n_1^{\alpha'}, n_2^{\alpha'}, \dots, n_L^{\alpha'} | \dots, n_j^\alpha - 1, \dots, n_i^\alpha + 1, \dots \rangle = \delta_{n_i^{\alpha'}, n_i^\alpha + 1} \delta_{n_j^{\alpha'}, n_j^\alpha - 1} \prod_{k \neq i,j} \delta_{n_k^{\alpha'}, n_k^\alpha} \quad (10)$$

where n_i^α is the number of particles on site i of the state $|\alpha\rangle$ and the product is carried over all sites k , excluding i and j . The elements of the kinetic operator then become:

$$H_1^{\alpha',\alpha} = - \sum_{i,j} t_{i,j} \sqrt{n_j^\alpha(n_j^\alpha + 1)} \delta_{n_i^{\alpha'}, n_i^\alpha + 1} \delta_{n_j^{\alpha'}, n_j^\alpha - 1} \prod_{k \neq i,j} \delta_{n_k^{\alpha'}, n_k^\alpha} \quad (11)$$

1.1.3 Worm operator

In the next section, it will be discussed in more detail how the partition function can be written as path integrals along the imaginary time direction. These paths, which will be known as worldlines, may have discontinuities along them. Worldline discontinuities will arise due to the insertion of bosonic creation or annihilation operators, which will be known as worm tails and heads, respectively. Here, we will define a "worm operator", related to the insertion or deletion of worm ends. The worm operator is defined as:

$$H_{\text{worm}} = -\eta \sum_i (b_i^\dagger + b_i) \quad (12)$$

where η is a tunable parameter known as the worm fugacity and the sum will be carried over all lattice sites. Sandwiching between Fock states, the matrix elements of the worm operator are obtained:

$$\langle \alpha' | H_{\text{worm}} | \alpha \rangle \equiv H_{\text{worm}}^{\alpha', \alpha} \quad (13)$$

In the derivation of the kinetic energy matrix elements $H_1^{\alpha', \alpha}$, the Fock states were rewritten explicitly in terms of site occupation numbers as $|\alpha\rangle = |n_1^\alpha, n_2^\alpha, \dots, n_L^\alpha\rangle$. Rewriting basis states in this way, the matrix elements of the worm operator become:

$$H_{\text{worm}}^{\alpha', \alpha} = -\eta \sum_i (\sqrt{n_i^\alpha + 1} \delta_{n_i^{\alpha'}, n_i^\alpha + 1} + \sqrt{n_i^\alpha} \delta_{n_i^{\alpha'}, n_i^\alpha - 1}) \prod_{k \neq i} \delta_{n_k^{\alpha'}, n_k^\alpha} \quad (14)$$

Eqs. (3), (11), and (14) give the diagonal, off-diagonal, and worm matrix elements of the Bose-Hubbard Hamiltonian (1). These elements will be necessary in order to sample the partition function of a Bose-Hubbard configuration via Path Integral Monte Carlo. In the next section, the path integral formulation of the partition will be discussed.

2 Partition function

The partition function is defined as:

$$\mathcal{Z} = \text{Tr } \rho = \text{Tr } e^{-\beta H}$$

where $e^{-\beta H} = \rho$ is the density matrix of the system and $|\psi_T\rangle$ is the trial state. The ground state can be exactly obtained by:

$$|\psi_0\rangle = \lim_{\beta \rightarrow \infty} e^{-\frac{\beta}{2} H} |\psi_T\rangle \quad (15)$$

where $\beta = \frac{1}{k_B T}$, H is the ground state Hamiltonian, and $|\psi_T\rangle$ is a trial wavefunction. Under this definition, the ground state weight Z_0 can then be approximated as the expectation

value of the density operator $e^{\beta H}$:

$$\mathcal{Z}_0 = \langle \psi_0 | \hat{I} | \psi_0 \rangle = \lim_{\beta \rightarrow \infty} \langle \psi_T | e^{-\beta H} | \psi_T \rangle \quad (16)$$

To save some typing effort in what follows, define the argument of the limit above as:

$$\mathcal{Z}_T \equiv \langle \psi_T | e^{-\beta H} | \psi_T \rangle \quad (17)$$

This "trial weight" \mathcal{Z}_T and hence the ground state weight \mathcal{Z} , can be sampled via Path Integral Monte Carlo (PIMC). To do this, \mathcal{Z}_T has to be rewritten in the path integral formulation.

2.0.1 Path integral representation of the partition function

Due to completeness of the wavefunction, the trial state $|\psi_T\rangle$ can be expanded as:

$$|\psi_T\rangle = \sum_{\alpha} C_{\alpha} |\alpha\rangle \quad (18)$$

where the C_{α} 's are complex expansion coefficients, and the sum is carried over all possible states $|\alpha\rangle$ of a conveniently chosen basis. For the Bose-Hubbard model, the basis that we will "conveniently choose" is the set of all configurations of N particles on a lattice of L sites (i.e, the Fock states). The trial weight becomes:

$$\mathcal{Z}_T = \sum_{\alpha_0, \alpha_1} C_{\alpha_0} C_{\alpha_1}^* \langle \alpha_0 | e^{-\beta H} | \alpha_1 \rangle \quad (19)$$

where each of the sums is carried over all Fock states. The state labels could be chosen arbitrarily, but with the power of hindsight, numerical subscripts have been used to distinguish the bra-ket pair, as it will ease the notation in the following steps. Nevertheless, keep in mind that both α_0 and α_1 will span the space of all Fock configurations, and are not just two basis states of the Hamiltonian.

In the interaction picture of quantum mechanics, the density operator can be expressed as:

$$e^{-\beta H} = e^{-\beta H_0} T_\tau e^{-\int_0^\beta d\tau_1 [H_1(\tau_1) + H_{\text{worm}}(\tau_1)]} \quad (20)$$

where T_τ is the imaginary time-ordering operator and $\tau = it/\hbar$ is the imaginary time. The integrand in the exponent is the interaction picture representation of the off-diagonal part of the Hamiltonian (kinetic and worm operators):

$$H_1(\tau_1) = e^{\tau_1 H_0} H_1 e^{-\tau_1 H_0} \quad (21)$$

$$H_{\text{worm}}(\tau_1) = e^{\tau_1 H_0} H_{\text{worm}} e^{-\tau_1 H_0} \quad (22)$$

where the kinetic and worm operators H_1 and H_{worm} , respectively are the off-diagonal parts of the Hamiltonian, and H_0 is the diagonal (interaction and chemical potential). The time-ordered exponential can be Taylor expanded as:

$$e^{-\int_0^\beta d\tau_1 H_1(\tau_1)} = \mathbb{1} - \int_0^\beta H_1(\tau_1) d\tau_1 + \int_0^\beta d\tau_1 \int_0^{\tau_1} d\tau_2 H_1(\tau_1) H_1(\tau_2) - \dots \quad (23)$$

Notice that the H_{worm} term has been dropped to save some space. It will be inserted at the end of the derivation.

Substituting the Taylor expansion into the trial weight \mathcal{Z}_T , it is seen that:

$$\begin{aligned} \mathcal{Z}_T = \sum_{\alpha_0, \alpha_1} C_{\alpha_0} C_{\alpha_1}^* e^{-\epsilon_{\alpha_0} \beta} \langle \alpha_0 | (& \\ \mathbb{1} - \int_0^\beta H_1(\tau_1) d\tau_1 + \int_0^\beta d\tau_1 \int_0^{\tau_1} d\tau_2 H_1(\tau_1) H_1(\tau_2) - \dots) | \alpha_1 \rangle & \end{aligned} \quad (24)$$

where ϵ_{α_0} is the an eigenvalue of H_0 , such that $H_0 |\alpha_0\rangle = \epsilon_{\alpha_0} |\alpha_0\rangle$. By evaluating the first few terms of the Taylor expansion, a generating formula for the trial weight \mathcal{Z}_T can be obtained.

The zeroth-order term is:

$$\begin{aligned}
\mathcal{Z}_T^{(0)} &= \sum_{\alpha_0, \alpha_1} C_{\alpha_0} C_{\alpha_1}^* e^{-\epsilon_{\alpha_0} \beta} \langle \alpha_0 | \mathbb{1} | \alpha_1 \rangle \\
&= \sum_{\alpha_0, \alpha_1} C_{\alpha_0} C_{\alpha_1}^* e^{-\epsilon_{\alpha_0} \beta} \langle \alpha_0 | \alpha_1 \rangle \\
&= \sum_{\alpha_0, \alpha_1} C_{\alpha_0} C_{\alpha_1}^* e^{-\epsilon_{\alpha_0} \beta} \delta_{\alpha_0, \alpha_1} \\
\mathcal{Z}_T^{(0)} &= \sum_{\alpha_0} |C_{\alpha_0}|^2 e^{-\epsilon_{\alpha_0} \beta}
\end{aligned} \tag{25}$$

First-order term:

$$\begin{aligned}
\mathcal{Z}_T^{(1)} &= - \sum_{\alpha_0, \alpha_1} C_{\alpha_0} C_{\alpha_1}^* \int_0^\beta d\tau_1 e^{-\epsilon_{\alpha_0} \beta} \langle \alpha_0 | H_1(\tau_1) | \alpha_1 \rangle \\
&= - \sum_{\alpha_0, \alpha_1} C_{\alpha_0} C_{\alpha_1}^* \int_0^\beta d\tau_1 e^{-\epsilon_{\alpha_0} \beta} \langle \alpha_0 | e^{\tau_1 H_0} H_1 e^{-\tau_1 H_0} | \alpha_1 \rangle \\
&= - \sum_{\alpha_0, \alpha_1} C_{\alpha_0} C_{\alpha_1}^* \int_0^\beta d\tau_1 e^{-\epsilon_{\alpha_0}(\beta - \tau_1)} e^{-\epsilon_{\alpha_1} \tau_1} \langle \alpha_0 | H_1 | \alpha_1 \rangle
\end{aligned} \tag{26}$$

Second-order term:

$$\begin{aligned}
\mathcal{Z}_T^{(2)} &= \sum_{\alpha_0, \alpha_2} C_{\alpha_0} C_{\alpha_2}^* \int_0^\beta d\tau_1 \int_0^{\tau_1} d\tau_2 e^{-\epsilon_{\alpha_0} \beta} \langle \alpha_0 | H_1(\tau_1) H_1(\tau_2) | \alpha_2 \rangle \\
&= \sum_{\alpha_0, \alpha_1, \alpha_2} C_{\alpha_0} C_{\alpha_2}^* \int_0^\beta d\tau_1 \int_0^{\tau_1} d\tau_2 e^{-\epsilon_{\alpha_0} \beta} \langle \alpha_0 | H_1(\tau_1) | \alpha_1 \rangle \langle \alpha_1 | H_1(\tau_2) | \alpha_2 \rangle \\
&= \sum_{\alpha_0, \alpha_1, \alpha_2} C_{\alpha_0} C_{\alpha_2}^* \int_0^\beta d\tau_1 \int_0^{\tau_1} d\tau_2 e^{-\epsilon_{\alpha_0} \beta} \langle \alpha_0 | e^{\tau_1 H_0} H_1 e^{-\tau_1 H_0} | \alpha_1 \rangle \langle \alpha_1 | e^{\tau_2 H_0} H_1 e^{-\tau_2 H_0} | \alpha_2 \rangle \\
\mathcal{Z}_T^{(2)} &= \sum_{\alpha_0, \alpha_1, \alpha_2} C_{\alpha_0} C_{\alpha_2}^* \int_0^\beta d\tau_1 \int_0^{\tau_1} d\tau_2 e^{-\epsilon_{\alpha_0}(\beta - \tau_1)} e^{-\epsilon_{\alpha_1}(\tau_1 - \tau_2)} e^{-\epsilon_{\alpha_2} \tau_2} \langle \alpha_0 | H_1 | \alpha_1 \rangle \langle \alpha_1 | H_1 | \alpha_2 \rangle
\end{aligned} \tag{27}$$

Proceeding in similar fashion, the Q -th term of \mathcal{Z}_T becomes:

$$\mathcal{Z}_T^{(Q)} = (-1)^Q \sum_{\alpha_0, \alpha_1, \dots, \alpha_Q} C_{\alpha_0} C_{\alpha_Q}^* e^{-\epsilon_{\alpha_Q} \tau_Q} \prod_{q=0}^Q \int_0^{\tau_{q-1}} d\tau_q e^{-\epsilon_{\alpha_{q-1}} (\tau_{q-1} - \tau_q)} \langle \alpha_{q-1} | H_1 | \alpha_q \rangle \quad (28)$$

where $\tau_0 = \beta > \tau_1 > \tau_2 > \dots > \tau_Q = 0$. Summing $\mathcal{Z}_T^{(Q)}$ over all Q from 0 to ∞ , the full expression for \mathcal{Z}_T is obtained:

$$\mathcal{Z}_T = \sum_{Q=0}^{\infty} \mathcal{Z}_T^{(Q)} \quad (29)$$

Recall from Eq. (16) that:

$$\mathcal{Z}_0 = \langle \psi_0 | \hat{I} | \psi_0 \rangle = \lim_{\beta \rightarrow \infty} \langle \psi_T | e^{-\beta H} | \psi_T \rangle = \lim_{\beta \rightarrow \infty} \mathcal{Z}_T \quad (30)$$

Finally, insert back the H_{worm} terms and the weight \mathcal{Z}_0 approximately becomes:

$$\mathcal{Z}_0 \approx \sum_{Q=0}^{\infty} (-1)^Q \sum_{\alpha_0, \alpha_1, \dots, \alpha_Q} C_{\alpha_0} C_{\alpha_Q}^* e^{-\epsilon_{\alpha_Q} \tau_Q} \prod_{q=1}^Q \int_0^{\tau_{q-1}} d\tau_q e^{-\epsilon_{\alpha_{q-1}} (\tau_{q-1} - \tau_q)} (H_1^{\alpha_{q-1}, \alpha_q} + H_{\text{worm}}^{\alpha_{q-1}, \alpha_q}) \quad (31)$$

where the off-diagonal elements $\langle \alpha_{q-1} | H_1 | \alpha_q \rangle$ and $\langle \alpha_{q-1} | H_{\text{worm}} | \alpha_q \rangle$ are given by Eq. (11) and Eq. (14), the diagonal elements ϵ_{α} are given by Eq. (3) and the approximation becomes exact in the limit $\beta \rightarrow \infty$.

3 Metropolis sampling

In this section, a brief walkthrough of the Metropolis-Hastings algorithm [1] will be given. First, the process of obtaining acceptance ratios that satisfy the Principle of Detailed Balance will be given. Then, the Metropolis-Hastings algorithm will be stated. The notes in this section follow the discussion in [2].

3.1 Deriving Metropolis acceptance ratios

The Principle of Detailed Balance states that in an equilibrium system, the number of transitions from a configuration x to a configuration x' , must be equal to the number of transitions from x' to x . This principle can be expressed as:

$$p(x)P(x \rightarrow x') = p(x')P(x' \rightarrow x) \quad (32)$$

where $p(x)$ is the steady state probability distribution, and $P(x \rightarrow x')$ is the probability of transitioning to x' conditional to original state x . Solving for the ratio of transition probabilities:

$$\frac{P(x \rightarrow x')}{P(x' \rightarrow x)} = \frac{p(x')}{p(x)} \quad (33)$$

The transition probability can be rewritten as a factor of proposal and acceptance probabilities:

$$P(x \rightarrow x') = g(x \rightarrow x')A(x \rightarrow x') \quad (34)$$

where $g(x \rightarrow x')$ is the probability of proposing an update that takes the state of the system from x to x' , and $A(x \rightarrow x')$ is the probability of accepting such update. Substituting the factored transition probabilities into Eq. (33):

$$\frac{g(x \rightarrow x')A(x \rightarrow x')}{g(x' \rightarrow x)A(x' \rightarrow x)} = \frac{p(x')}{p(x)} \quad (35)$$

The ratio of acceptance probabilities becomes:

$$\frac{A(x \rightarrow x')}{A(x' \rightarrow x)} = \frac{p(x')g(x' \rightarrow x)}{p(x)g(x \rightarrow x')} \equiv R \quad (36)$$

Depending on the value of R , there are various ways in which the acceptance probabilities can be chosen, such that they satisfy Eq. (36).

If $R \leq 1$:

$$A(x \rightarrow x') = R \text{ and } A(x' \rightarrow x) = 1$$

If $R > 1$:

$$A(x \rightarrow x') = 1 \text{ and } A(x' \rightarrow x) = 1/R$$

The above selections can be summarized as:

$$A(x \rightarrow x') = \min\{1, R\} \text{ and } A(x' \rightarrow x) = \min\{1, 1/R\} \quad (37)$$

As part of Metropolis sampling, proposed configurations will be accepted with the probabilities in Eq. (37).

4 Lattice Worm Algorithm (WA) Updates

In this section, a set of ergodic lattice worm updates is introduced. First, an explanation of how each update changes the system is given. Then, a walkthrough of the decisions that comprise each update will be given, including the probabilities for each decision's outcome. Finally, the Metropolis conditions are derived or the direct sampling explained, depending on the update.

4.0.1 Insert worm

The insert worm update creates a particle on a flat region of a worldline, then destroys it after a certain time, also inside the same flat region. Formally, the particle is created by acting on the state at that imaginary time with the bosonic creation operator (worm tail) and annihilated by acting with the bosonic annihilation operator (worm head). An antiworm can instead be inserted by first inserting the worm head and then the tail. In other words, an antiworm will first annihilate a particle and create one at a later time inside the flat region. Propose update if there are no worm ends present. The update proceeds as follows:

0. Do with probability p_{iw}
1. Randomly choose an integer $i \in [0, L - 1]$, where L is the number of sites on the lattice.
The i^{th} site will be chosen with probability $1/L$.
2. Randomly choose an integer $k \in [0, N_{\text{flats}} - 1]$, where N_{flats} is the number of flat regions on site i . The flat region will be chosen with probability $1/N_{\text{flats}}$
3. Count the number of particles n_{flat} on the flat region and check if inserting an antiworm is possible:
 - (a) If $n_{\text{flat}} = 0$: Only a worm can be inserted with probability $p_{\text{type}} = 1$
 - (b) Else: A worm or antiworm can be inserted with probability $p_{\text{type}} = 1/2$
4. Calculate the diagonal energy difference $dV = \epsilon_w - \epsilon$, where ϵ_w is the diagonal energy of the segment of path inside the flat with more particles. Based on the sign, choose the length of the worm or antiworm τ_{worm} :
 - (a) if $dV \neq 0$: Draw τ_{worm} from $p_{\tau_{\text{worm}}} = dV e^{-dV \tau_{\text{worm}}} / (1 - e^{-dV \tau_{\text{flat}}})$
 - (b) Else: Choose τ_{worm} with probability $p_{\tau_{\text{worm}}} = \frac{1}{\tau_{\text{flat}}}$

where $\tau_{\text{flat}} = \tau_{\text{next}} - \tau_{\text{prev}}$ is the length of the flat interval.
5. Randomly select a real number $\tau = \tau_{\text{prev}} + U(0, 1) * (\tau_{\text{flat}} - \tau_{\text{worm}})$, where τ_{prev} is the lower bound of the flat region. The probability of inserting the worm (antiworm) tail (head) at τ is $1/(\tau_{\text{flat}} - \tau_{\text{worm}})$.

4.0.2 Delete worm

The delete worm update is proposed when there are two worm ends present on the same site and same flat interval. The update will be attempted with probability p_{dw} .

The Metropolis condition for the insert/delete update pair becomes:

$$\begin{aligned}
R_{\text{insert}} &= \frac{W'}{W} \frac{p(\alpha' \rightarrow \alpha)}{p(\alpha \rightarrow \alpha')} \\
&= \eta^2 n_i^{\alpha_w} e^{-dV \tau_{\text{worm}}} \cdot \frac{L \cdot N_{\text{flats}} \cdot (\tau_{\text{flat}} - \tau_{\text{worm}}) \frac{p_{\text{dw}}}{p_{\text{iw}}}}{p_{\tau_{\text{worm}}} \cdot p_{\text{type}}} \quad (38)
\end{aligned}$$

Recalling that $p_{\tau_{\text{worm}}}$ depends on the value of the diagonal energy difference $dV = \epsilon_w - \epsilon$, the Metropolis condition can be rewritten as a piece-wise defined function:

$$R_{\text{insert}} = \begin{cases} \eta^2 n_i^{\alpha_w} \frac{(1 - e^{-dV \tau_{\text{flat}}})}{dV} \cdot \frac{L \cdot N_{\text{flats}} \cdot (\tau_{\text{flat}} - \tau_{\text{worm}}) \frac{p_{\text{dw}}}{p_{\text{iw}}}}{p_{\text{type}}} & dV \neq 0 \\ \eta^2 n_i^{\alpha_w} e^{-dV \tau_{\text{worm}}} \cdot \frac{L \cdot N_{\text{flats}} \cdot \tau_{\text{flat}} \cdot (\tau_{\text{flat}} - \tau_{\text{worm}}) \frac{p_{\text{dw}}}{p_{\text{iw}}}}{p_{\text{type}}} & dV = 0 \end{cases} \quad (39)$$

and $R_{\text{delete}} = 1/R_{\text{insert}}$.

4.0.3 Timeshift

The timeshift update is proposed when there is at least one worm end present. A worm end is selected randomly, then moved backward or forward in the imaginary time direction. The update proceeds as follows:

1. Choose a worm end with probability $p_{\text{wormend}} = 1/2$ or $p_{\text{wormend}} = 1$, depending if there's two or one worm ends, respectively.
2. Calculate $dV = \epsilon_w - \epsilon$.
 - (a) if $dV \neq 0$: Draw τ' from $p_{\tau} = dV e^{-dV \tau'} / (1 - e^{-dV \tau_{\text{flat}}})$
 - (b) Else: Draw τ' from $U(0, 1) * \tau_{\text{flat}}$, i.e with probability $p_{\tau} = 1/\tau_{\text{flat}}$

The Metropolis condition becomes:

$$R_{\text{timeshift}} = \begin{cases} 1 & dV \neq 0 \\ e^{-dV(\tau'_h - \tau_h)} & dV = 0 \end{cases} \quad (40)$$

The above derivation assumes timeshift of a worm head. In the case of a tail shift:

$$R_{\text{timeshift}} = \begin{cases} 1 & dV \neq 0 \\ e^{-dV(\tau_t - \tau'_t)} & dV = 0 \end{cases} \quad (41)$$

4.0.4 Insert worm from $\tau = 0$

At $T = 0$, open boundary conditions (OBC) are imposed in the imaginary time direction. This allows for the insertion of worms from the imaginary time edges, that is $\tau = 0$ and $\tau = \beta$. This update can only be done if there is at most one other worm end present. To insert a worm or antiworm from the $\tau = 0$ edge, we proceed as follows.

0. Do with probability p_{iwz}
1. Choose site with probability $p = 1/L$
2. Count particles on the first flat to determine the type of worm to be inserted.
 - (a) If $n = 0$: propose to insert a worm from $\tau = 0$ with probability $p_{\text{type}} = 1$
 - (b) Else: propose to insert worm or antiworm from $\tau = 0$ with $p_{\text{type}} = 1/2$
3. Calculate $dV = \epsilon_w - \epsilon$.
 - (a) if $dV \neq 0$: Draw τ from $p_{\tau_h} = dV e^{-dV\tau_h} / (1 - e^{-dV\tau_{\text{flat}}})$
 - (b) Else: Choose τ with probability $p_{\tau_h} = 1/\tau_{\text{flat}}$

4.0.5 Delete worm from $\tau = 0$

The delete worm from zero update can only be done if there's at least one worm end on the worldline configuration, and that also lies on the first flat of the site. The worm end is chosen and deleted from the configuration. The update proceeds as follows

0. Do with probability p_{dwz}

1. Count how many worm ends are present near zero.

(a) If only one worm end is present, choose it with probability $p_{\text{wormend}} = 1$.

(b) Else, choose the worm end randomly with probability $p_{\text{wormend}} = 1/2$

The Metropolis condition of the insert/delete from zero update becomes:

$$\begin{aligned} R_{\text{insertZero}} &= \frac{W'}{W} \frac{p(\alpha' \rightarrow \alpha)}{p(\alpha \rightarrow \alpha')} \\ &= \eta \sqrt{n_i^{\alpha_w}} \frac{C_{\alpha_w}}{C_\alpha} e^{-dV\tau_h} \cdot \frac{L \cdot p_{\text{wormend}}}{p_{\tau_h} \cdot p_{\text{type}}} \frac{p_{\text{dwz}}}{p_{\text{iwz}}} \end{aligned} \quad (42)$$

Which can be expressed as a piece-wise defined function, depending on the value of dV :

$$R_{\text{insertZero}} = \begin{cases} \eta \sqrt{n_i^{\alpha_w}} \frac{C_{\alpha_w}}{C_\alpha} \frac{(1 - e^{-dV\tau_{\text{flat}}})}{dV} \cdot \frac{L \cdot p_{\text{wormend}}}{p_{\text{type}}} \frac{p_{\text{dwz}}}{p_{\text{iwz}}} & dV \neq 0 \\ \eta \sqrt{n_i^{\alpha_w}} \frac{C_{\alpha_w}}{C_\alpha} e^{-dV\tau_h} \cdot \frac{L \cdot \tau_{\text{flat}} \cdot p_{\text{wormend}}}{p_{\text{type}}} \frac{p_{\text{dwz}}}{p_{\text{iwz}}} & dV = 0 \end{cases} \quad (43)$$

The above derivation assumes insertion of a worm near zero. In the case of an antiworm near zero, the ratio of weights becomes instead:

$$\frac{W'}{W} = \eta \sqrt{n_i^{\alpha_w}} \frac{C_\alpha}{C_{\alpha_w}} e^{-(\epsilon_w - \epsilon)(-\tau_t)} \quad (44)$$

Notice that the only difference with the case of a worm insertion is that $\tau_h \rightarrow -\tau_t$. This implies that in the case that $dV \neq 0$, the length of the antiworm is drawn from:

$$p_{\tau_t} = dV e^{dV\tau_t} / (1 - e^{-dV\tau_{\text{flat}}}) \quad (45)$$

The Metropolis condition when inserting an antiworm near zero becomes:

$$R_{\text{insertZero}} = \begin{cases} \eta \sqrt{n_i^{\alpha_w}} \frac{C_{\alpha_w}}{C_\alpha} \frac{(1 - e^{-dV\tau_{\text{flat}}})}{dV} \cdot \frac{L \cdot p_{\text{wormend}}}{p_{\text{type}}} \frac{p_{\text{dwz}}}{p_{\text{iwz}}} & dV \neq 0 \\ \eta \sqrt{n_i^{\alpha_w}} \frac{C_{\alpha_w}}{C_\alpha} e^{dV\tau_t} \cdot \frac{L \cdot \tau_{\text{flat}} \cdot p_{\text{wormend}}}{p_{\text{type}}} \frac{p_{\text{dwz}}}{p_{\text{iwz}}} & dV = 0 \end{cases} \quad (46)$$

and $R_{\text{deleteZero}} = 1/R_{\text{insertZero}}$.

4.0.6 Insert worm from $\tau = \beta$

This update is analogous to inserting a worm end from $\tau = 0$. The only difference is that the worm end is proposed to be inserted in the last flat of a site. The Metropolis condition

4.0.7 Delete worm from $\tau = \beta$

This update can only be proposed if there is at least one worm end on the last flat of a site. Otherwise, the update is analogous to deleting from $\tau = 0$.

4.1 Weight ratios of updates

The weight of a worldline configuration can be read off from the partition function Eq. (31):

INSERT WEIGHT EXPRESSION HERE

For each the moves in the ergodic set of updates discussed, the rhe ratio of post and pre update weights need to be calculated. These will show up in the detailed balance equation and will thus be necessary to get the Metropolis condition for each update. In this section, the weigh ratio for each update is shown.

4.2 Summary of weight ratios

1. Insert: $\frac{W'}{W} = \eta^2 n_i^{\alpha_w} e^{-(\epsilon_w - \epsilon)(\tau_h - \tau_t)}$
2. Delete: $\frac{W'}{W} = 1/(\eta^2 n_i^{\alpha_w} e^{-(\epsilon_w - \epsilon)(\tau_h - \tau_t)})$
3. Timeshift
 - (a) Shift head: $\frac{W'}{W} = e^{-(\epsilon_w - \epsilon)(\tau'_h - \tau_h)}$
 - (b) Shift tail: $\frac{W'}{W} = e^{-(\epsilon_w - \epsilon)(\tau_t - \tau'_t)}$
4. Insert from $\tau = 0$

- (a) Worm: $\frac{W'}{W} = \eta \sqrt{n_i^{\alpha_w}} \frac{C_{\alpha_w}}{C_\alpha} e^{-(\epsilon_w - \epsilon)\tau_h}$
- (b) Antiworm: $\frac{W'}{W} = \eta \sqrt{n_i^{\alpha_w}} \frac{C_\alpha}{C_{\alpha_w}} e^{-(\epsilon_w - \epsilon)(-\tau_t)}$

5. Delete from $\tau = 0$

- (a) Worm: $\frac{W'}{W} = 1/(\eta \sqrt{n_i^{\alpha_w}} \frac{C_{\alpha_w}}{C_\alpha} e^{-(\epsilon_w - \epsilon)\tau_h})$
- (b) Antiworm: $\frac{W'}{W} = 1/(\eta \sqrt{n_i^{\alpha_w}} \frac{C_\alpha}{C_{\alpha_w}} e^{-(\epsilon_w - \epsilon)(-\tau_t)})$

6. Insert from $\tau = \beta$

- (a) Worm: $\frac{W'}{W} = \eta \sqrt{n_i^{\alpha_w}} \frac{C_{\alpha_w}}{C_\alpha} e^{-(\epsilon_w - \epsilon)(\beta - \tau_t)}$
- (b) Antiworm: $\frac{W'}{W} = \eta \sqrt{n_i^{\alpha_w}} \frac{C_\alpha}{C_{\alpha_w}} e^{-(\epsilon_w - \epsilon)(\tau_h - \beta)}$

7. Delete from $\tau = \beta$

- (a) Worm: $\frac{W'}{W} = 1/(\eta \sqrt{n_i^{\alpha_w}} \frac{C_{\alpha_w}}{C_\alpha} e^{-(\epsilon_w - \epsilon)(\beta - \tau_t)})$
- (b) Antiworm: $\frac{W'}{W} = 1/(\eta \sqrt{n_i^{\alpha_w}} \frac{C_\alpha}{C_{\alpha_w}} e^{-(\epsilon_w - \epsilon)(\tau_t - \beta)})$

4.3 Summary of attempt probability ratios

Let $p(\alpha \rightarrow \alpha')$ be the probability of attempting an update that takes the system from configuration α to α' . As part of the detailed balance equation of each move, the ratio of attempt probabilities for the reverse and forward updates are needed. In this section, the ratio of attempt probabilities are shown for each move.

1. Insert: $\frac{p(\alpha' \rightarrow \alpha)}{p(\alpha \rightarrow \alpha')} = \frac{p_{dw}}{p_{iw}} \cdot \frac{1}{\Theta} \frac{L \cdot N_{\text{flats}} \cdot (\tau_{\text{flat}} - \tau_{\text{worm}})}{p_{\text{type}}} \cdot e^{(\epsilon_w - \epsilon)(\tau_h - \tau_t)}$
2. Delete: $\frac{p(\alpha' \rightarrow \alpha)}{p(\alpha \rightarrow \alpha')} = 1/(\frac{p_{dw}}{p_{iw}} \cdot \frac{1}{\Theta} \frac{L \cdot N_{\text{flats}} \cdot (\tau_{\text{flat}} - \tau_{\text{worm}})}{p_{\text{type}}} \cdot e^{(\epsilon_w - \epsilon)(\tau_h - \tau_t)})$
3. Timeshift
 - (a) Shift head: $\frac{p(\alpha' \rightarrow \alpha)}{p(\alpha \rightarrow \alpha')} = e^{(\epsilon_w - \epsilon)(\tau'_h - \tau_h)}$
 - (b) Shift tail: $\frac{p(\alpha' \rightarrow \alpha)}{p(\alpha \rightarrow \alpha')} = e^{(\epsilon_w - \epsilon)(\tau_t - \tau'_t)}$

4. Insert from $\tau = 0$

$$\begin{aligned} \text{(a) worm: } \frac{p(\alpha' \rightarrow \alpha)}{p(\alpha \rightarrow \alpha')} &= \frac{p_{\text{dwz}}}{p_{\text{iwz}}} \frac{1}{\Theta} \frac{L \cdot p_{\text{wormend}}}{p_{\text{type}}} e^{(\epsilon_w - \epsilon) \tau_h} \\ \text{(b) antiworm: } \frac{p(\alpha' \rightarrow \alpha)}{p(\alpha \rightarrow \alpha')} &= \frac{p_{\text{dwz}}}{p_{\text{iwz}}} \frac{1}{\Theta} \frac{L \cdot p_{\text{wormend}}}{p_{\text{type}}} e^{(\epsilon_w - \epsilon)(-\tau_t)} \end{aligned}$$

5. Delete from $\tau = 0$

$$\begin{aligned} \text{(a) worm: } \frac{p(\alpha' \rightarrow \alpha)}{p(\alpha \rightarrow \alpha')} &= 1 / \left(\frac{p_{\text{dwz}}}{p_{\text{iwz}}} \frac{1}{\Theta} \frac{L \cdot p_{\text{wormend}}}{p_{\text{type}}} e^{(\epsilon_w - \epsilon) \tau_h} \right) \\ \text{(b) antiworm: } \frac{p(\alpha' \rightarrow \alpha)}{p(\alpha \rightarrow \alpha')} &= 1 / \left(\frac{p_{\text{dwz}}}{p_{\text{iwz}}} \frac{1}{\Theta} \frac{L \cdot p_{\text{wormend}}}{p_{\text{type}}} e^{(\epsilon_w - \epsilon)(-\tau_t)} \right) \end{aligned}$$

6. Insert from $\tau = \beta$

$$\begin{aligned} \text{(a) worm: } \frac{p(\alpha' \rightarrow \alpha)}{p(\alpha \rightarrow \alpha')} &= \frac{p_{\text{dwz}}}{p_{\text{iwz}}} \frac{1}{\Theta} \frac{L \cdot p_{\text{wormend}}}{p_{\text{type}}} e^{(\epsilon_w - \epsilon)(\beta - \tau_t)} \\ \text{(b) antiworm: } \frac{p(\alpha' \rightarrow \alpha)}{p(\alpha \rightarrow \alpha')} &= \frac{p_{\text{dwz}}}{p_{\text{iwz}}} \frac{1}{\Theta} \frac{L \cdot p_{\text{wormend}}}{p_{\text{type}}} e^{(\epsilon_w - \epsilon)(\tau_h - \beta)} \end{aligned}$$

7. Delete from $\tau = \beta$

$$\begin{aligned} \text{(a) worm: } \frac{p(\alpha' \rightarrow \alpha)}{p(\alpha \rightarrow \alpha')} &= 1 / \left(\frac{p_{\text{dwz}}}{p_{\text{iwz}}} \frac{1}{\Theta} \frac{L \cdot p_{\text{wormend}}}{p_{\text{type}}} e^{(\epsilon_w - \epsilon)(\beta - \tau_t)} \right) \\ \text{(b) antiworm: } \frac{p(\alpha' \rightarrow \alpha)}{p(\alpha \rightarrow \alpha')} &= 1 / \left(\frac{p_{\text{dwz}}}{p_{\text{iwz}}} \frac{1}{\Theta} \frac{L \cdot p_{\text{wormend}}}{p_{\text{type}}} e^{(\epsilon_w - \epsilon)(\tau_h - \beta)} \right) \end{aligned}$$

4.4 Summary of Metropolis conditions

The Metropolis condition of each update is given by:

$$R = \frac{W'}{W} \frac{p(\alpha' \rightarrow \alpha)}{p(\alpha \rightarrow \alpha')} \quad (47)$$

In this section, the Metropolis condition of each update is shown.

1. Insert: $R = \frac{p_{\text{dw}}}{p_{\text{iw}}} \cdot \frac{1}{\Theta} \frac{L \cdot N_{\text{flats}} \cdot (\tau_{\text{flat}} - \tau_{\text{worm}})}{p_{\text{type}}} \cdot \eta^2 n_i^{\alpha_w}$
2. Delete: $R = 1 / \left(\frac{p_{\text{dw}}}{p_{\text{iw}}} \cdot \frac{1}{\Theta} \frac{L \cdot N_{\text{flats}} \cdot (\tau_{\text{flat}} - \tau_{\text{worm}})}{p_{\text{type}}} \cdot \eta^2 n_i^{\alpha_w} \right)$
3. Timeshift:

(a) Shift head: $R = 1$

(b) Shift tail: $R = 1$

4. Insert from $\tau = 0$

(a) worm: $R = \frac{p_{\text{dwz}}}{p_{\text{iwz}}} \frac{1}{\Theta} \frac{L \cdot p_{\text{wormend}}}{p_{\text{type}}} \eta \sqrt{n_i^{\alpha_w} \frac{C_{\alpha_w}}{C_\alpha}}$

(b) antiworm: $R = \frac{p_{\text{dwz}}}{p_{\text{iwz}}} \frac{1}{\Theta} \frac{L \cdot p_{\text{wormend}}}{p_{\text{type}}} \eta \sqrt{n_i^{\alpha_w} \frac{C_\alpha}{C_{\alpha_w}}}$

5. Delete from $\tau = 0$

(a) worm: $R = 1 / \left(\frac{p_{\text{dwz}}}{p_{\text{iwz}}} \frac{1}{\Theta} \frac{L \cdot p_{\text{wormend}}}{p_{\text{type}}} \eta \sqrt{n_i^{\alpha_w} \frac{C_{\alpha_w}}{C_\alpha}} \right)$

(b) antiworm: $R = 1 / \left(\frac{p_{\text{dwz}}}{p_{\text{iwz}}} \frac{1}{\Theta} \frac{L \cdot p_{\text{wormend}}}{p_{\text{type}}} \eta \sqrt{n_i^{\alpha_w} \frac{C_\alpha}{C_{\alpha_w}}} \right)$

6. Insert from $\tau = \beta$

(a) worm: $R = \frac{p_{\text{dwb}}}{p_{\text{iwb}}} \frac{1}{\Theta} \frac{L \cdot p_{\text{wormend}}}{p_{\text{type}}} \eta \sqrt{n_i^{\alpha_w} \frac{C_{\alpha_w}}{C_\alpha}}$

(b) antiworm: $R = \frac{p_{\text{dwb}}}{p_{\text{iwb}}} \frac{1}{\Theta} \frac{L \cdot p_{\text{wormend}}}{p_{\text{type}}} \eta \sqrt{n_i^{\alpha_w} \frac{C_\alpha}{C_{\alpha_w}}}$

7. Delete from $\tau = \beta$

(a) worm: $R = 1 / \left(\frac{p_{\text{dwb}}}{p_{\text{iwb}}} \frac{1}{\Theta} \frac{L \cdot p_{\text{wormend}}}{p_{\text{type}}} \eta \sqrt{n_i^{\alpha_w} \frac{C_{\alpha_w}}{C_\alpha}} \right)$

(b) antiworm: $R = 1 / \left(\frac{p_{\text{dwb}}}{p_{\text{iwb}}} \frac{1}{\Theta} \frac{L \cdot p_{\text{wormend}}}{p_{\text{type}}} \eta \sqrt{n_i^{\alpha_w} \frac{C_\alpha}{C_{\alpha_w}}} \right)$

where,

$$\Theta = \begin{cases} dV / (1 - e^{-dV \tau_{\text{flat}}}), & dV \neq 0 \\ 1 / \tau_{\text{flat}}, & dV = 0 \end{cases} \quad (48)$$

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