

Probabilistic representation of fermionic lattice systems

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We describe an exact Feynman-Kac type formula to represent the dynamics of fermionic lattice systems. In this approach the real time or Euclidean time dynamics is expressed in terms of the stochastic evolution of a collection of Poisson processes. From this formula we derive a family of algorithms for Monte Carlo simulations, parametrized by the jump rates of the Poisson processes.

Quantum Monte Carlo methods are powerful techniques for the numerical evaluation of the properties of quantum lattice systems. In the case of fermion systems [1–4] there are special features connected with the anticommutativity of the variables involved. In a recent paper [5] progress has been made by providing an exact probabilistic representation for the dynamics of a Hubbard model. Here we illustrate the basic formula while for details we refer to [5].

Let us consider the Hubbard Hamiltonian

$$H = - \sum_{i=1}^{|\Lambda|} \sum_{j=i+1}^{|\Lambda|} \sum_{\sigma=\uparrow\downarrow} \eta_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + \sum_{i=1}^{|\Lambda|} \gamma_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow}, \quad (1)$$

where $\Lambda \subset \mathbb{Z}^d$ is a finite d -dimensional lattice with cardinality $|\Lambda|$, $\{1, \dots, |\Lambda|\}$ some total ordering of the lattice points, and $c_{i\sigma}$ the usual anticommuting destruction operators at site i and spin index σ . In this paper, we are interested in evaluating the matrix elements $\langle \mathbf{n}' | e^{-Ht} | \mathbf{n} \rangle$ where $\mathbf{n} = (n_{1\uparrow}, n_{1\downarrow}, \dots, n_{|\Lambda|\uparrow}, n_{|\Lambda|\downarrow})$ are the occupation numbers taking the values 0 or 1. The total number of fermions per spin component is a conserved quantity, therefore we consider only configurations \mathbf{n} and \mathbf{n}' such that $\sum_{i=1}^{|\Lambda|} n'_{i\sigma} = \sum_{i=1}^{|\Lambda|} n_{i\sigma}$

for $\sigma = \uparrow\downarrow$. In the following we shall use the mod 2 addition $n \oplus n' = (n + n') \bmod 2$.

Let $\Gamma = \{(i, j), 1 \leq i < j \leq |\Lambda| : \eta_{ij} \neq 0\}$ and $|\Gamma|$ its cardinality. For simplicity, we will assume that $\eta_{ij} = \eta$ if $(i, j) \in \Gamma$ and $\gamma_i = \gamma$. By introducing

$$\lambda_{ij\sigma}(\mathbf{n}) \equiv \langle \mathbf{n} \oplus \mathbf{1}_{i\sigma} \oplus \mathbf{1}_{j\sigma} | c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} | \mathbf{n} \rangle = (-1)^{n_{i\sigma} + \dots + n_{j-1\sigma}} [n_{j\sigma} (n_{i\sigma} \oplus 1) - n_{i\sigma} (n_{j\sigma} \oplus 1)], \quad (2)$$

where $\mathbf{1}_{i\sigma} = (0, \dots, 0, 1_{i\sigma}, 0, \dots, 0)$, and

$$V(\mathbf{n}) \equiv \langle \mathbf{n} | H | \mathbf{n} \rangle = \gamma \sum_{i=1}^{|\Lambda|} n_{i\uparrow} n_{i\downarrow}, \quad (3)$$

the following representation holds

$$\langle \mathbf{n}' | e^{-Ht} | \mathbf{n} \rangle = \mathbf{E} (\delta_{\mathbf{n}', \mathbf{n} \oplus \mathbf{N}^t} \mathcal{M}^t) \quad (4)$$

$$\mathcal{M}^t = \exp \left\{ \sum_{(i,j) \in \Gamma} \sum_{\sigma=\uparrow\downarrow} \int_{[0,t]} \log [\eta \rho^{-1} \times \lambda_{ij\sigma}(\mathbf{n} \oplus \mathbf{N}^s)] dN_{ij\sigma}^s - \int_0^t V(\mathbf{n} \oplus \mathbf{N}^s) ds + 2|\Gamma| \rho t \right\}. \quad (5)$$

Here, $\{N_{ij\sigma}^t\}$, $(i, j) \in \Gamma$, is a family of $2|\Gamma|$ independent Poisson processes with parameter ρ

and $\mathbf{N}^t = (N_{1\uparrow}^t, N_{1\downarrow}^t, \dots, N_{|\Lambda|\uparrow}^t, N_{|\Lambda|\downarrow}^t)$ are $2|\Lambda|$ stochastic processes defined as

$$N_{k\sigma}^t = \sum_{(i,j) \in \Gamma: i=k \text{ or } j=k} N_{ij\sigma}^t. \quad (6)$$

We remind that a Poisson process N^t with parameter ρ is a jump process characterized by the following probabilities:

$$P(N^{t+s} - N^t = k) = \frac{(\rho s)^k}{k!} e^{-\rho s}. \quad (7)$$

Its trajectories are piecewise-constant increasing integer-valued functions continuous from the left. The stochastic integral $\int dN^t$ is just an ordinary Stieltjes integral

$$\int_{[0,t)} f(s, N^s) dN^s = \sum_{k: s_k < t} f(s_k, N^{s_k}),$$

where s_k are random jump times having probability density $p(s) = \rho e^{-\rho s}$. Finally, the symbol $\mathbf{E}(\dots)$ is the expectation of the stochastic functional within braces. We emphasize that a similar representation holds for the real time matrix elements $\langle \mathbf{n}' | e^{-iHt} | \mathbf{n} \rangle$.

Summarizing, we associate to each $\eta_{ij} \neq 0$ a link connecting the sites i and j and assign to it a pair of Poisson processes $N_{ij\sigma}^t$ with $\sigma = \uparrow\downarrow$. Then, we assign to each site i and spin component σ a stochastic process $N_{i\sigma}^t$ which is the sum of all the processes associated with the links incoming at that site and having the same spin component. A jump in the link process $N_{ij\sigma}^t$ implies a jump in both the site processes $N_{i\sigma}^t$ and $N_{j\sigma}^t$. Equations (4) and (5) are immediately generalizable to non identical parameters η_{ij} and γ_i . In this case, it may be convenient to use Poisson processes $N_{ij\sigma}^t$ with different parameters $\rho_{ij\sigma}$.

In order to construct an efficient algorithm for evaluating (4-5), we start by observing that the functions $\lambda_{ij\sigma}(\mathbf{n} \oplus \mathbf{N}^s)$ vanish when the occupation numbers $n_{i\sigma} \oplus N_{i\sigma}^s$ and $n_{j\sigma} \oplus N_{j\sigma}^s$ are equal. We say that for a given value of σ the link ij is active at time s if $\lambda_{ij\sigma}(\mathbf{n} \oplus \mathbf{N}^s) \neq 0$. We shall see in a moment that only active links are relevant. Let us consider how the stochastic integral in (5) builds up along a trajectory defined by considering the time ordered succession of jumps in the

family $\{N_{ij\sigma}^t\}$. The contribution to the stochastic integral in the exponent of (5) at the first jump time of a link, for definiteness suppose that the link $i_1 j_1$ with spin component σ_1 jumps first at time s_1 , is

$$\log [\eta \rho^{-1} \lambda_{i_1 j_1 \sigma_1}(\mathbf{n} \oplus \mathbf{N}^{s_1})] \theta(t - s_1),$$

where $\mathbf{N}^{s_1} = \mathbf{0}$ due the assumed left continuity. Therefore, if the link $i_1 j_1 \sigma_1$ was active at time 0 we obtain a finite contribution to the stochastic integral otherwise we obtain $-\infty$. If $s_1 \geq t$ we have no contribution to the stochastic integral from this trajectory. If $s_1 < t$ a second jump of a link, suppose $i_2 j_2$ with spin component σ_2 , can take place at time $s_2 > s_1$ and we obtain a contribution

$$\log [\eta \rho^{-1} \lambda_{i_2 j_2 \sigma_2}(\mathbf{n} \oplus \mathbf{N}^{s_2})] \theta(t - s_2).$$

The analysis can be repeated by considering an arbitrary number of jumps. Of course, when the stochastic integral is $-\infty$, which is the case when some $\lambda = 0$, there is no contribution to the expectation. The other integral in (5) is an ordinary integral of a piecewise constant bounded function.

We now describe the algorithm. The only trajectories to be considered are those associated to jumps of the active links. This guarantees conservation of the total number of fermions per spin component. The active links can be determined after each jump by inspecting the occupation numbers of the sites in the set Γ according to the rule that the link ij is active for the spin component σ if $n_{i\sigma} + n_{j\sigma} = 1$. We start by determining the active links in the initial configuration \mathbf{n} assigned at time 0 and make an extraction with uniform distribution to decide which of them jumps first. We then extract the jump time s_1 according to the probability density $p_{A_1}(s) = A_1 \rho \exp(-A_1 \rho s)$ where A_1 is the number of active links before the first jump takes place. The contribution to \mathcal{M}^t at the time of the first jump is therefore, up to the factor $\exp(-2|\Gamma|\rho t)$,

$$\begin{aligned} & \eta \rho^{-1} \lambda_{i_1 j_1 \sigma_1}(\mathbf{n} \oplus \mathbf{N}^{s_1}) e^{-V(\mathbf{n} \oplus \mathbf{N}^{s_1}) s_1} \\ & \times e^{-(2|\Gamma| - A_1) \rho s_1} \theta(t - s_1) \\ & + e^{-V(\mathbf{n} \oplus \mathbf{N}^t) t} e^{-(2|\Gamma| - A_1) \rho t} \theta(s_1 - t), \end{aligned}$$

where $\exp[-(2|\Gamma| - A_1)\rho s]$ is the probability that the $2|\Gamma| - A_1$ non active links do not jump in the time interval s . The contribution of a given trajectory is obtained by multiplying the factors corresponding to the different jumps until the last jump takes place later than t . For a given trajectory we thus have

$$\begin{aligned} \mathcal{M}^t = & \prod_{k \geq 1} \left[\eta \rho^{-1} \lambda_{i_k j_k \sigma_k}(\mathbf{n} \oplus \mathbf{N}^{s_k}) \right. \\ & \times e^{[A_k \rho - V(\mathbf{n} \oplus \mathbf{N}^{s_k})](s_k - s_{k-1})} \theta(t - s_k) \\ & \left. + e^{[A_k \rho - V(\mathbf{n} \oplus \mathbf{N}^t)](t - s_{k-1})} \theta(s_k - t) \right]. \quad (8) \end{aligned}$$

Here, $A_k = A(\mathbf{n} \oplus \mathbf{N}^{s_k})$ is the number of active links in the interval $(s_{k-1}, s_k]$ and $s_0 = 0$. Note that the exponentially increasing factor $\exp(2|\Gamma|\rho t)$ in (5) cancels out in the final expression of \mathcal{M}^t . The analogous expression of \mathcal{M}^t for real times is simply obtained by replacing $\eta \rightarrow i\eta$ and $\gamma \rightarrow i\gamma$. The algorithm can be improved by the usual methods of reconfiguration and importance sampling.

In principle, the algorithms parametrized by ρ are all equivalent as (4-5) holds for any choice of the Poisson rates. However, since we estimate the expectation values with a finite number of trajectories, this may introduce a systematic error. It can be shown that the best performance is obtained for the natural choice $\rho \sim \eta$ independently of the interaction strength. In this case our algorithm coincides with the Green function Monte Carlo method in the limit when the latter becomes exact as discussed in [5].

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