The International Journal of Advanced Research In Multidisciplinary Sciences
(IJARMS)
Volume 2 Issue 1, 2019

Quantum Monte Carlo Investigations for The Hubbard Model

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Abstract:

Simulations of Quantum Monte ***Carlo*** *(QMC) are a powerful way of collecting knowledge about quantum mechanical systems with close interactions. The chapter demonstrates how the Monte Carlo quantum method is used for finite temperature systems that are highly correlated and that the Hubbard model can be represented as well.The partition function is broken down by means of a transformation from Trotter—Suzuki (TS). The relationship is decoupled by Hubbard—Stratonovich transformation.There are brief mention of the problems caused by numerical instabilities and the problem of negative signs due to Monte Carlo's sampling technology.*

Keywords: Quantum Monte **Carlo**, Hubbard Model, QMC, Hubbard Interaction.

Introduction

The Hubbard Model:

The dynamic conduct of Hubbard-like Hamiltonians cannot be identified andSimulation without simplifications in a single chapter.Thus the diagrams in this article show the moving and interacting "classical particles," not taking into account collective phenomena essential for the "real" physics of the problem.

A general Hamiltonian can be written as (spin indices are omitted) for a system of N-electrons which interact in real space through Coulomb interaction into an external potential Ue^'

$$H^{\text{general}} = \underbrace{-\frac{\hbar}{2m}\sum_{i=1}^{N}\nabla_i^2}_{E_{\text{Kin}}} + \underbrace{\frac{1}{2}\sum_{i\neq j=1}^{N}\frac{e^2}{|r_i - r_j|}}_{E_{\text{Int}}} + \underbrace{\sum_{i=1}^{N}V^{\text{ext}}(r_i)}_{E_{\text{Pot}}} \quad , \qquad \ldots\ldots\ldots\ldots\ldots\ldots(1)$$

Where *r*; in actual space reflects electron co-ordinates. For solid electrons, ri is not permanent; only some "lattic points" can be occupied and the contact between Coulomb is screened. To define the tightly bound approach of intracting electrons,

1. Use the formal occupation number to allow distinct locations as particulate positions only;
2. neglect the external ability to invariantly translate our system.
3. Only maintain the contact on-site. We have theHubbardHamiltonian

$$H^{\mathrm{Hub}} = \underbrace{-t\sum_{i,j,s} c^{+}_{i,s}c_{j,s}}_{E_{\mathrm{Kin}}} + \underbrace{U\sum_{i} n_{i\uparrow}n_{i\downarrow}}_{E_{\mathrm{Int}}} \underbrace{-\mu\sum_{i}(n_{i\uparrow}+n_{i\downarrow})}_{\text{Chem. Pot}} \quad , \qquad \text{.....(2)}$$

Where operator c,, creates spin s particles at the sites I and c;„ the operator annihilates a spin s particle at the sites i. rii„ = c c„,, is the number operator, the occupancy number of which is a site z occupational with a spin s fermion.The overview index is available for all grid sites, The word cxiv exists between adjacent sites i, y, while the electrons with opposite spines on the same site are felt through Hubbard on-site contact H.w.The final term in (2) is similar in conventional physics to —PM suggesting the injection of particles into the system if y > 0, while particles are p< 0 from the system, y=0.5 refers to the system half filled (nit) = (oil) = 0.5. Fig. 1 displays the two cases with Hamiltonian (1) respectively Hamiltonian (2).

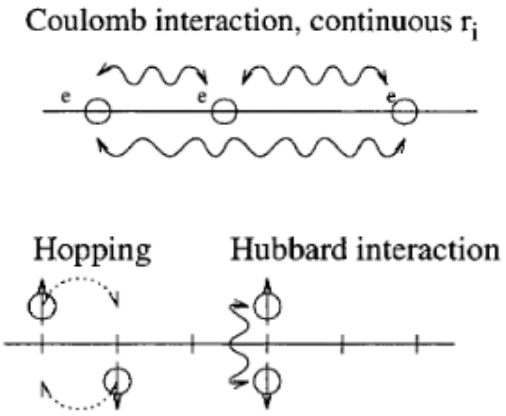

Figure1: Simplified electron behavior showed few Hamiltonian the(1), **Hamiltonian**the(2) **shown right**.The diagrams are one-dimensional two-dimensional simplifications.

The following units I=1 (GB=) represent the energy and temperature. The word 'hopping' in dynamic space is diagonal, in real space is the term for interaction. Disturbance rises are also only true for such doping regimes.

The Hubbard Hamiltonian is the generic Hamiltoni-ans model. As the Ising model is used for "spin" systems, it is in its simplest form, the workhorse for highly correlated electrons. It can however be generalized via:

- Additional interactions; the nearest-neighbor in the extended Hubbard model

  (nn)interactionsV; , „ *n„ n1* , (z is nearest neighbor to *1)* areincluded.
- Further hopping situations, t — t' hopping; hopping between the nearest

  (nun) neighboring sites change the density and kinetic energy of the states.

Hubbard model and QMC simulations:

A basic model for researching one of the main problems in materials science is the Hubbard model:How do solid electron interactions create such characteristics as magnetism, superconductivity and the transitions of metal-insulators?In our lecture we introduce the Hubbard model and explain the quantum Monte Carlo (QMC) to study multiple electron systems.The following lectures describe the QMC simulation machine kernels.

A Hamiltonian describes the two-dimensional models of the Hubbard [8, 9] we are studying:

$$\mathcal{H} = \mathcal{H}_K + \mathcal{H}_\mu + \mathcal{H}_V, \quad \text{.....(3)}$$

where H_K, H_μ and H_V stand for kinetic energy, chemical energy and potential energy, respectively, and are defined as

$$\mathcal{H}_K = -t \sum_{\langle i,j\rangle,\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}),$$

$$\mathcal{H}_\mu = -\mu \sum_i (n_{i\uparrow} + n_{i\downarrow})$$

$$\mathcal{H}_V = U \sum_i (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2})$$

And

- The spaces of the lattice is labeled by *i* and *j*.*i*, *j* represents a couple of nearest-neighbor sites in the net, and shows the electrons that are hopping only to the nearest neighboring sites,
- the operators $c^{\dagger}_{i\sigma}$ and $c_{i\sigma}$are the fermion formation and the annihila-tion of electron operators with spin-up ($\sigma = \uparrow$) or spin-down ($\sigma = \downarrow$), respectively, are located at the *i*th.
- lattice location.$n_{i\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma}$ are the number operators that count the electrons of spin σ on site *i*.
- *t* is the kinetic electron energy hopping parameter and is calculated by a superposition of atomic wave functions at neigh-boring sites.
- *U* is the abominable interaction of coulomb on a common grid of electrons. For the site *i*have two electrons and a local repulsion between electric electrons, the word $U\, n_{i\uparrow}n_{i\downarrow}$ tutorial reflects an energy cost *U*.
- μ is an electron number (or density) control potential chemical parameter.
- Notice that we take a half-filled band into consideration. The Hamil-tonian is therefore expressly written in symmetrical form in particle-hole form.

Hubbard model with no hopping:

Consider the Hubbard Model, that is, there is only a site and there is no hopping, $t = 0$. The Hamiltonian *H* is therefore

$$\mathcal{H} = U(n_{\uparrow} - \frac{1}{2})(n_{\downarrow} - \frac{1}{2}) - \mu(n_{\uparrow} + n_{\downarrow}).$$

The orthonormal autonomy of operator n_{σ} can be checked that the individual statesψ_i of the hamiltonian *H*: are:

$$\mathcal{H} : |\cdot\rangle = \tfrac{U}{4}|\cdot\rangle, \qquad |\uparrow\rangle = \left(\tfrac{U}{4} - (\mu + \tfrac{U}{2})\right)|\uparrow\rangle,$$
$$|\downarrow\rangle = \left(\tfrac{U}{4} - (\mu + \tfrac{U}{2})\right)|\downarrow\rangle, |\uparrow\downarrow\rangle = \left(\tfrac{U}{4} - 2\mu\right)|\uparrow\downarrow\rangle.$$

The Hamiltonian *H* is diagonalized according to the base$\{\psi_i\}$:

$$\mathcal{H} \longrightarrow (\langle\psi_i|\mathcal{H}|\psi_j\rangle) = \begin{bmatrix} \frac{U}{4} & & \\ & \frac{U}{4} - (\mu + \frac{U}{2}) & \\ & & \frac{U}{4} - (\mu + \frac{U}{2}) \\ & & & \frac{U}{4} - 2\mu \end{bmatrix}.$$

Consequently, $e^{-\beta H}$is diagonalized from the operator:

$$e^{-\beta\mathcal{H}} \longrightarrow e^{-\frac{U\beta}{4}} \mathrm{diag}\left(1, e^{\beta(U/2+\mu)}, e^{\beta(U/2+\mu)}, e^{2\mu\beta}\right).$$

The partition function Z is transformed

$$\mathcal{Z} = \mathrm{Tr}(e^{-\beta\mathcal{H}}) = \sum_i \langle\psi_i|e^{-\beta\mathcal{H}}|\psi_i\rangle \longrightarrow Z = e^{-\frac{U\beta}{4}}\left(1 + 2e^{\left(\frac{U}{2}+\mu\right)\beta} + e^{2\mu\beta}\right)$$

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