The International Journal of Advanced Research In Multidisciplinary Sciences
(IJARMS)
Volume 3 Issue 2, Nov. 2020

A Study on Determinantal Quantum Monte Carlo: Preliminaries

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Abstract

Preliminary performance evaluations PPE assessments are important in the development of useful guidance for proper software development decisions on different computational platforms. In order to provide useful guidance for correct software design choice, preliminary performance evaluations (PPE) on various computational platforms is necessary.In the present article, we analyse the performance of quantitative kernels of the determinant quantum Monte Carlo (DQMC) of two common computer processors: multi-core CPU and GPU. They demonstrate how these approaches can be used for a number of models, including Hubbard Hamiltonians, standard Anderson, Kondo lattice and problems with impurities as well as hardcore bosons and the Heisenberg model.

Keywords: *Quantum Monte Carlo, QMC, Determinant Quantum Monte Carlo, DQMC, Hubbard Hamiltonians.*

Introduction

In one dimension only the Hubbard model is correctly soluble by means of Bethe ansatz; however, correlation functions cannot be explicitly given. In the higher dimensions, approximation systems must be used with the extraction knowledge about closely correlated fermions having proven critical numerical techniques such as Quantum Monte Carlo (QMC).

Since the first classic systems method of Monte Carlo had been developed in the early 1950s[1-3], a number of QMC algorithms were suggested. Their rating is different, and it depends on the factor you want to classify.For example, they can be categorised by whether the degrees of freedom lie in the continuum or on a lattice; whether it is a soil State or a final temperature framework; whether it is versatile or projective; or whether it has even been applied according to specifics, such as the implementation of an auxiliary field, or the creation of a green function through the power new method.The literature has an excellent general overview of these algorithms, including Refs. [4,5], we focus here on the actual specifics of the grand-canonic formulation, with supporting fields that lead to fermionic determinants. The implementations and enhancements made over the years will

receive special attention.We will also primarily consider the Hubbard model, but we will not analyse the findings obtained at length. Instead we will offer the reader illustrative references for more detailed research, and we apologies for the lack of many relevant papers dictated by the need to concentrate the discussion on this particular QMC implementation rather than on the Hubbard.

According to the intent of this study, the fundamental components of Monte Carlo simulations, demonstrated for "classical" spins, are introduced in Sec. In this way, we have the opportunity to carry out to the attention of the unrealized reader, before embarking on the more elaborated quantum formalism, the value of detailed data analyses common to both traditional and quantum systems. The Secretary would then be debating provisional manipulations, approximations and the natural presence in the context of the Green functions.In Sec., we define both the update process and the broad range of average amounts available to detect different device physical properties.We address then two of the key difficulties present in the simple algorithm presented so far the "minus-sign problem" that is still unresolved (sec.), and low-temperature instabilities (sec.), which are two solutions that have proved effective. Sec. 7 then outlines observations and several insights.

Determinantal Quantum Monte Carlo: Preliminaries

The fact that various terms in Hamiltonian do not commute is the manifestation of quantum effects. For the Hubbard model, there are no contact and hopping terms, and also no hopping terms with the same site communicate with each other. The particles thus lose their individuality since they are essentially associated.

One way to overcome these non-commuting aspects[6] is to remember that in the Hamiltonian it includes two-line terms (hopping and chemicals) and fourword operators (the interaction term). Terms may be trivial in the former category but not in the latter category. When the major partition function is determined,

$$\mathcal{Z} = \mathcal{T}re^{-\beta\mathcal{H}}, \quad \text{.....(1)}$$

Where as usual, $\mathcal{T}$ r represents a total of all particle numbers and occupations on the site, a quartic term must be put in a bilinear shape.

To this end, we are separating the exponentials by means of the decomposition scheme Suzuki-Trotter[11], based upon the fact that

$$e^{\Delta\tau(A+B)} = e^{\Delta\tau A}e^{\Delta\tau B} + \mathcal{O}\left[(\Delta\tau)^2\right][A,B], \quad \text{.....(2)}$$

For the non-commuting generic operators*A* or *B*. Calling $\mathcal{K}$ and $\mathcal{V}$, The bilinear and the Hubbard Hamiltonian quartic terms respectively, We join the small parameter Dτ by b = M Dτ and we use the formula Suzuki-Trotter

$$e^{-\beta(\mathcal{K}+\mathcal{V})} = \left(e^{\Delta\tau\mathcal{K}+\Delta\tau\mathcal{V}}\right)^M = \\ = \left(e^{\Delta\tau\mathcal{K}}e^{\Delta\tau\mathcal{V}}\right)^M + \mathcal{O}\left[(\Delta\tau)^2 U\right]. \quad \text{.....(3)}$$

A path integral analogy of Quantum Mechanics indicates that the above procedure is the *imaginary-time* interval (0,b) which is divided into *M* slices separated by Dτ.

As this whole process can take a lot of time, at least one can verify that the results are not too sensitive to *D*$\tau$by measuring two *D*τ values and comparing the results.

After the exponentials have been divided, we can now practise the fourth terms in $\mathcal{V}$. We remember firstly a popular trick to transform the operator's square into an operator's own exponential transformation, known as the transformation Hubbard-Stratonovich (HS).

$$e^{\frac{1}{2}A^2} \equiv \sqrt{2\pi}\int_{-\infty}^{\infty} dx e^{-\frac{1}{2}x^2 - xA}, \quad \text{.....(4)}$$

However, in the argument of exponentiality squares of the operators must be shown before a transformation of this kind can refer to the quartic term of the Hubbard Hamiltonian.Since you've got fermions n_σ^2 º n_s = 0,1 (Here we have omitted indices for the simplification of notation), The following identity – local magnetization, *m* º *n* – *n*–, and of local responsibility, *n* º *n* + *n*– – is going to suit our objectives:

$$n_\uparrow n_\downarrow = -\frac{1}{2}m^2 + \frac{1}{2}n, \quad \text{.....(5a)}$$

$$n_\uparrow n_\downarrow = \frac{1}{2}n^2 - \frac{1}{2}n, \quad \text{.....(5b)}$$

$$n_\uparrow n_\downarrow = \frac{1}{4}n^2 - \frac{1}{4}m^2, \quad \text{.....(5c)}$$

It is worth noting the following points on Eqs. (5), for the transformation of the HS: (i) for each squared operator shown above on the RHS's, an auxiliary field shall be introduced;

(ii) when Eqs is respectively, the auxiliary fields are connected to the local magnetization and to local load. (5a) and (5b); (iii) Eqs shall be included. For repulsive and attractive versions (5a) and (5b) are used respectively.

Rather than the continuous Eq. subsidiary domain. (4), dealing with *discrete*Ising variables, *s* = ±1 [7]. is more convenient in simulations. Eq's inspired. (4), Eq. Usage. (5a), it's clear to see that taking into accounts^2 º 1,

$$e^{-U\Delta\tau n_\uparrow n_\downarrow} = \frac{1}{2} e^{-\frac{U\Delta\tau}{2} n} \sum_{s=\pm 1} e^{-s\lambda m} =$$

$$= \frac{1}{2} \sum_{s=\pm 1} \prod_{\sigma=\uparrow,\downarrow} e^{-\left(\sigma s\lambda + \frac{U\Delta\tau}{2}\right) n_\sigma}, U > 0,$$

……..(6)

where the grouping of the two fermion spin channels factorises in the latter equality, s = +,– referring to the respective s = , ¯), and

$$\cosh \lambda = e^{|U|\Delta\tau/2}.$$

……..(7)

The coupling to the charge [Eq.] would be attractive. (5b)] shall be used to prevent complicated HS transformation;

$$e^{|U|\Delta\tau n_\uparrow n_\downarrow} = \frac{1}{2} \sum_{s=\pm 1} \prod_{\sigma=\uparrow,\downarrow} e^{\left(s\lambda + \frac{|U|\Delta\tau}{2}\right)\left(n_\sigma - \frac{1}{2}\right)} U < 0,$$

…….. (8)

Eq. also gives with l. There was a mistake (7).

In repellents or attractive situations, the HS transformations replace an on-site interaction with a fluctuating field combined with the magnetization or the load. Consequently, in the previous case, but not in the latter the exponential argument depends directly on s. As we see below the absence of the 'minus-sign problem' in the attractive case is the cause of this significant difference.

We now substitute Eqs. for on-site interaction on each position in the space-time grid. (6) or (8), which correspond to the form requested in which the exponential appears only in bilinear terms. We get the disgusting situation

$$Z = \left(\frac{1}{2}\right)^{L^d M} \operatorname*{Tr}_{\{s\}} \mathcal{T}r \prod_{\ell=M}^{1} \prod_{\sigma=\uparrow,\downarrow} e^{-\Delta\tau \sum_{i,j} c^\dagger_{i\sigma} K_{ij} c_{j\sigma}} e^{-\Delta\tau \sum_i c^\dagger_{i\sigma} V_i^\sigma(\ell) c_{i\sigma}},$$

…….. (9)

The product from $\ell = M$ to 1 represents only that earlier 'times' appears to the right, where the traces are over Ising fields and over fermion occupancies at all locations. The index ℓ of the time-slice is displayed through the $s_i(\ell)$ region.

$$V_i^\sigma(\ell) = \frac{1}{\Delta\tau} \lambda \sigma s_i(\ell) + \left(\mu - \frac{U}{2}\right),$$

…….... (10)

which are the components of $N_s \times N_s$ Matrix diagonal $V^s(\ell)$. You must also have the $N_s \times N_s$ Matrix hopping K, with objects

$$K_{ij} = \begin{cases} -t & \text{if } i \text{ and } j \text{ are nearest neighbours,} \\ 0 & \text{otherwise} \end{cases}$$

…….... (11)

For e.g., one has an $L \times L$ matrix in one dimension and with periodic boundary conditions,

$$\mathsf{K} = \begin{pmatrix} 0 & -t & 0 & \cdots & 0 & -t \\ -t & 0 & -t & \cdots & 0 & 0 \\ 0 & -t & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ -t & 0 & \cdots & 0 & -t & 0 \end{pmatrix}.$$

…….... (12)

The fermions can be traced out of Eq. with bilinear forms in the exponential. (9) in accordance with the Appendices *A* and *B* innovations. The Eq. (124), the spin indices have been reintroduced and $e^{-\mathrm{D}\,\tau^{\mathrm{h}\,s(\ell)}}\,\mathrm{o}\,e^{-\mathrm{D}\,\tau^{\mathrm{K}}}\,e^{-\mathrm{D}\,\tau^{\mathrm{V}\,s\,(\ell)}}$, has been established,

$$\mathcal{Z} = \left(\frac{1}{2}\right)^{L^d M} \operatorname*{Tr}_{\{s\}} \prod_{\sigma} \det\left[1 + \mathsf{B}_M^\sigma \mathsf{B}_{M-1}^\sigma \ldots\ \mathsf{B}_1^\sigma\right],$$

…….... (13)

Where did we describe

$$\mathsf{B}_\ell^\sigma \equiv e^{-\Delta\tau \mathsf{K}} e^{-\Delta\tau \mathsf{V}^\sigma(\ell)},$$

…….... (14)

where the dependency on the auxiliary spins Ising has not been written specifically but it is understandable because they arrive via matrix $\mathrm{V}^{\mathrm{s}}(\ell)$. Presentation

$$\mathsf{O}^\sigma(\{s\}) \equiv 1 + \mathsf{B}_M^\sigma \mathsf{B}_{M-1}^\sigma \ldots\ \mathsf{B}_1^\sigma,$$

…….... (15)

Finally, we come to

$$\mathcal{Z} = \left(\frac{1}{2}\right)^{L^d M} \operatorname*{Tr}_{\{s\}} \det \mathsf{O}^{\uparrow}(\{s\}) \cdot \det \mathsf{O}^{\downarrow}(\{s\}) = \\ = \operatorname*{Tr}_{\{s\}} \rho(\{s\}),$$

…….... (16)

where a final 'density matrix'is defined by the effective equality, r({s}).

The great partition function was then represented as a sum over the spins of a determinant product. When the quantity under the Tr is positive, the value sampling of the Ising configurations could be

used as a Boltzmann weight. In fact, for some configurations the product of the determinants can actually be negative, leading to the 'minus-sign problem'; see sec. 5.

There is a strong need for a further approach from Eq. To apply the structure mentioned above. (14): an exponential hopping matrix needs to be evaluated, which in the general case, is neither analytically simple nor numerically efficient.When we look at a one-dimensional structure again we see the different powers of K as Eq. gives. (12), several different matrices are generated. But a 'checkerboard break-up' can be introduced by writing

$$K = K_x^{(a)} + K_x^{(b)}, \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (17)$$

The $K^{(a)}$ involves settings from 1 to 2, 3 to 4, ¼while $K^{(b)}$ involves settings from 2 to 3, 4 to 5,¼. We now invoke the decomposition scheme of Suzuki-Trotter

$$e^{-\Delta\tau K} = e^{-\Delta\tau K_x^{(a)}} e^{-\Delta\tau K_x^{(b)}} + \mathcal{O}\left[(\Delta\tau)^2\right], \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (18)$$

This leads to the same order of systemic mistakes as before. This option of break-up has also the power to$K_x^{(\alpha)}$a = *a,b,*become multiples of the matrix of identity or we end up with a simple term,

$$e^{-\Delta\tau K_x^{(\alpha)}} = K_x^{(\alpha)} \sinh(\Delta\tau t) + 1 \cosh(\Delta\tau t), \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (19)$$

This makes numerical calculations very simple. Eq. division. (28) can be widespread as follows in three dimensions

$$e^{-\Delta\tau K} = e^{-\Delta\tau K_z^{(a)}} e^{-\Delta\tau K_y^{(a)}} e^{-\Delta\tau K_x^{(a)}} e^{-\Delta\tau K_z^{(b)}} e^{-\Delta\tau K_y^{(b)}} e^{-\Delta\tau K_x^{(b)}} + \mathcal{O}\left[(\Delta\tau)^2\right], \qquad \ldots\ldots\ldots\ldots \quad (20)$$

where the separation is like that for the one-dimensional case in any cartesian path. Finally, we need to discuss the average measurement of values. Their equal-'time' correlation function is for two operators *A* and *B.*

$$\langle AB \rangle = \frac{1}{Z} \operatorname{Tr}_{\{s\}} \mathcal{T} r \left[AB \prod_{\ell\sigma} e^{-\Delta\tau K} e^{-\Delta\tau V^{\sigma}(\ell)} \right]. \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (21)$$

If we now describe the average fermion - or Green's - for a particular HS field configuration

$$\langle AB\rangle_{\{s\}} \equiv \frac{1}{\rho(\{s\})}\mathcal{T}r\left[AB\prod_{\ell\sigma}e^{-\Delta\tau K}e^{-\Delta\tau V^{\sigma}(\ell)}\right],$$

…….... (22)

The role of correlation will be

$$\langle AB\rangle = \frac{1}{Z}\mathrm{Tr}_{\{s\}}\langle AB\rangle_{\{s\}}\,\rho(\{s\}).$$

…….... (23)

The importance of the functions of the Green in simulations should be emphasised at this point. Second, Eq. Firstly. (23), by sampling the corresponding feature green over HS configurations weighted by r({s}), the average value of an operator is obtained straightforwardly.Secondly, as it will become evident in Sec., the single particle Green's function, á c_{is} $c^{\dagger}_{j\sigma}$ñ $_{\{s\}}$, plays a central role in the updating process itself. In Appendix C we obtain this quantity as the element **ij** of a $N_s \times N_s$ matrix [5,8]:

$$\langle c_{i\sigma}c^{\dagger}_{j\sigma}\rangle_{\{s\}} = \left[\left(1+B^{\sigma}_{M}B^{\sigma}_{M-1}\ldots B^{\sigma}_{1}\right)^{-1}\right]_{ij},$$

…….... (24)

That is once again, in a numerical computational form. Thirdly, the fermions only work with the auxiliary fields in the current method, so that Wick's [20] theorem has *for a fixed HS configuration* [5,8,9]; the Green two-piece function is then readily given for the one-piece function as

$$\langle c^{\dagger}_{i1}c_{i2}c^{\dagger}_{i3}c_{i4}\rangle_{\{s\}} = \langle c^{\dagger}_{i1}c_{i2}\rangle_{\{s\}}\langle c^{\dagger}_{i3}c_{i4}\rangle_{\{s\}} + \langle c^{\dagger}_{i1}c_{i4}\rangle_{\{s\}}\langle c_{i2}c^{\dagger}_{i3}\rangle_{\{s\}},$$

…….... (25)

Where the indicators involve spin, but since both and ¯ spin channels [*c.f.* Eq. (22)], if the spins are different, thesefermion mean are zero. Therefore, any average interest value is determined in relation to the functions of the single-particle Green's.

Uniform correlation functions are also significant, as can be seen. In the 'Heisenberg picture' we define the operator as

$$a(\ell) \equiv a(\tau) = e^{\tau\mathcal{H}}ae^{-\tau\mathcal{H}},\ \tau \equiv \ell\Delta\tau,$$

…….... (26)

so the first time is set $\tau = D\tau$ with this discernment, or $a^{\square}(\ell)^{1}[a(\ell)]^{\square}$. In Appendix D, we demonstrate that unequal-time Green's function, for $\ell_1 > \ell_2$, is given by [8]

$$G^{\sigma}_{ij}(\ell_1;\ell_2) \equiv \langle c_{i\sigma}(\ell_1)c^{\dagger}_{j\sigma}(\ell_2)\rangle_{\{s\}} = [B^{\sigma}_{\ell_1}B^{\sigma}_{\ell_1-1}\dots B^{\sigma}_{\ell_2+1}g^{\sigma}(\ell_2+1)]_{ij} \quad \text{.......................... (27)}$$

where the ℓ-th time slice function matrix of the Green's is calculated as

$$g^{\sigma}(\ell) \equiv [1 + A^{\sigma}(\ell)]^{-1}, \quad \text{.......................... (28)}$$

with

$$A^{\sigma}(\ell) \equiv B^{\sigma}_{\ell-1}B^{\sigma}_{\ell-2}\dots B^{\sigma}_{1}B^{\sigma}_{M}\dots B^{\sigma}_{\ell}. \quad \text{.......................... (29)}$$

In order for the B's products to be taken in Eqs. the reading should be found (24), (27), or (29); in Eq. (27), The product runs from in particular ℓ_2+1 to ℓ_1, or not cyclically as in Eq. (29). In addition, for a given setup {s} The functions of Green's show a time-slice dependence of the HS spins, which is represented by Eq. (28); they're now getting (approximately) Equal over several configurations after averaging.

We also identify for the future

$$\tilde{g}^{\sigma}_{ij} \equiv [1 - g]_{ij}, \text{ and } \tilde{G}^{\sigma}_{ij} \equiv [1 - G]_{ij}. \quad \text{.......................... (30)}$$

Conclusion:

For fermionics, we have tested the Monte Carlo Determinant Quantum technique. This approach has developed tremendously since over 20 years ago, the pioneering proposal by Blankenbecler, Scalapino and Sugar[6].Stabilization techniques permitted the measurement of a variety of quantities at very low temperatures, but the minus-sign problem still plagues the simulations, restricting a full analysis over a large range of band fillings and coupling constants.

In this regard, it should be said that this under-signing issue is also caused by other QMC applications, such as ground-state algorithms (see Ref. [5]). A significant contribution would be an effective solution to this problem.

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