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Title: Boosting determinant quantum Monte Carlo with submatrix updates: Unveiling the phase diagram of the 3D Hubbard model

Dear Editor,

Thank you very much for the editorial assessment and forwarding the report from the respected referees on November 28th.

Below are our point-to-point responses to the suggestions from the respected referees, and we have made corresponding changes in the revised manuscript. With these, we would humbly like to resubmit our manuscript to SciPost Physics.

Sincerely,
Fanjie Sun and Xiao Yan Xu

Response to the first referee's report

First referee : *Although the article is very technical, providing such technical details is important for any researcher who wants to write their own DQMC code. Furthermore, understanding the physics of the Hubbard model is an important challenge in condensed-matter physics. It has become very clear in recent times that such an understanding goes hand in hand with technical developments / improvements in numerical techniques. That's why I am recommending publication. But before fully accepting the manuscript, I would like the following points to be addressed:*

The authors call their "innovative approach" a "generalized submatrix updating algorithm" because it can handle extended interactions and zero temperature. However, for the standard finite-temperature Hubbard model, which is the main model studied here, the introduction does not clearly explain, in my opinion, what has been done before and what is new. What's the difference with previous submatrix updating schemes for the finite-T half-filled Hubbard model (that couldn't go up to such large lattice sizes)? This is not clear from the current version of the manuscript

Reply: Thank you for your careful reading and important comments. We apologize for any lack of clarity in distinguishing our work from previous efforts.

While submatrix updates were originally developed for Hirsch-Fye QMC with onsite interactions at finite temperatures (Ref.1), and the original paper noted that extension to DQMC would be straightforward, a comprehensive implementation and application in DQMC has not been widely documented in the literature. To the best of our knowledge, there are no previous reports of submatrix updating schemes being implemented in DQMC for the finite-temperature half-filled Hubbard model - this likely explains why such large lattice sizes were not achieved before. Our work provides the first comprehensive application of submatrix updates in DQMC, with complete implementation details that enable simulations of the half-filled Hubbard model on lattices up to 8,000 sites.

We use the term "generalized" because our implementation extends beyond the original scope of submatrix updates by incorporating extended interactions and zero temperature calculations. To better clarify these points and distinguish our contributions from previous work, we have revised both the abstract and introduction accordingly.

First referee : *On page 3, the authors write "As this additional overhead is implemented with Level 1 BLAS, its time cost can surpass the time cost for the update of Green's function in practical calculation if one increase nd, as shown in Fig. 4." But for the values of nd shown in Fig. 4, this doesn't seem to be the case. That's why I found this sentence somewhat confusing.*

Reply: Thank you for your careful observation. You are correct - we made a typographical error in the reference. The statement refers to Fig. 3, not Fig. 4, where one can clearly see that due to the additional overhead, the update-ratio time surpasses the Green's function update time in the delayed update scheme as n_d increases. We have corrected this reference in the revised manuscript.

First referee : *It seems that the lattice sizes that were reached prior to this work were large enough to obtain a good estimate of the Néel temperature (using finite size scaling by crossing analysis). It is mentioned that previously one could go up to N=1000, or L=10. It's not very clear from the figures that going significantly beyond L=10 implies a significant improvement in the calculation of T_c. Could the authors indicate how much moving to larger lattice sites has decreased the error bar on T_c, which is what matters in the end. A related question: are there other quantities for which the effect of finite size is more important?*

Reply: Thank you for this insightful observation about finite-size effects. While it's true that three-dimensional systems generally show smaller finite-size effects compared to their two-dimensional counterparts, our ability to simulate systems up to $L = 20$ reveals important corrections to previously reported results.

Our finite-size scaling analysis demonstrates that the critical temperatures obtained using larger system sizes (up to $L = 20$) are systematically lower than those derived from systems limited to $L \leq 10$, as shown in Table. R1. This finding has direct experimental implications, particularly for cold atom simulations: researchers need to achieve lower temperatures than previously thought to observe antiferromagnetic ordering.

The finite-size effect is particularly pronounced at smaller U/t values. For example, at $U/t = 4$, our calculated critical temperature is more than 5% lower than previously reported values. This systematic difference becomes more significant when considering critical exponents, which are crucial for identifying universality classes. Our analysis of the critical exponent ν shows larger uncertainty for smaller U/t values, as shown in Fig. R2, consistent with the enhanced finite-size effects in this regime - an observation that aligns with the second referee's comments.

These findings underscore the importance of accessing larger system sizes, not just for more precise T_c

determinations, but especially for accurate characterization of critical phenomena and universality classes in different coupling regimes.

TABLE R1: The Néel temperature of the 3D half-filled Hubbard model on a cubic lattice.

U/t	T_c/t ($L \leq 10$)	T_c/t ($L \leq 10$, Staudt's data)	T_c/t ($L \leq 20$)
4	0.198(20)	0.20	0.185(24)
6	0.314(12)	0.31	0.2977(45)
8	0.339(9)	0.34	0.3336(42)
10	0.318(16)	0.32	0.3094(54)
12	0.283(7)	0.29	0.2779(20)

TABLE R2: The ν of the 3D half-filled Hubbard model on a cubic lattice for data collapse.

U/t	ν ($L \leq 10$)	ν ($L \leq 20$)
4	0.692(18)	0.703(6)
6	0.695(16)	0.704(5)
8	0.698(10)	0.704(4)
10	0.703(8)	0.706(2)
12	0.704(5)	0.707(1)

First referee : *The paper focuses on a static property of the Hubbard model, in order to determine the Néel temperature. What about dynamical properties of the system? Is it expected that one could also go up to L=20?*

Reply: Thank you again for your questions and we are pleased to explain the issue. The unequal-time Green's functions can be used to calculate dynamic properties of the system and we can obtain the unequal-time Green's function by applying the time evolution matrix on the equal-time Green's function, which is similar to propagating in the DQMC. The Trotter decomposition can be used for propagating, its computational complexity is $O(\beta N^2)$, which is much smaller than the complexity $O(\beta N^3)$ during the update process. Therefore, there is no problem to measure the dynamical properties up to $L = 20$.

Response to the second referee's report

Second referee : *Add reference Phys. Rev. B 99, 125145 (2019)*

Reply: We thank you for your insightful suggestions and recommendation for the paper to be publishable in SciPost Physics. We have carefully read this article. Not only is it related to our research, but it also broadens our perspective. We have cited it in the revised version of our manuscript.

Second referee : *As for the application, the authors look into the Hubbard model at half-filling on the cubic lattice, and determine the Néel temperature in terms as a function of the Hubbard U. I agree that the* *universality class is the 3D O(3) one. However, I think that the paper could benefit from a discussion of why this is so. The point is that at T_N the charge degrees of freedom are not gaped such as that one has to find an argument why they can be omitted in the critical theory. My naive understanding is that at T_N the charge excitations decay exponentially such that one can safely omit them in the critical theory. Given this conjecture, one can understand why corrections to scaling are more important in the weak coupling limit. This would stem for the fact that at weak coupling T_N is smaller, there is no pseudo gap, and the charge correlation length at T_N is longer at weak than at intermediate coupling*

Reply: Thank you for your insightful comment regarding the O(3) universality class and the role of charge degrees of freedom at the Néel temperature. We agree that a more detailed discussion of this important physics was needed. We have addressed this by adding a new section in the appendix (Appendix G) where we explicitly demonstrate how the charge degrees of freedom influence the critical behavior.

Your physical intuition about the charge excitations is indeed correct. To quantitatively support this picture, we have calculated the charge correlation length near the critical temperature for different interaction strengths and system sizes. The charge correlation shows exponential decay with distance. Importantly, our results show that at weaker coupling, the charge correlation length is longer, consistent with your understanding that corrections to scaling become more prominent in the weak coupling regime. The new results presented in Fig. R1 (Fig. 15 in the revised manuscript) provide clear evidence: as U/t decreases, the correlation length increases, indicating a smaller charge gap and thus stronger finite-size effects. This quantitative analysis provides solid support for your suggested physical mechanism and helps clarify why the transition belongs to the O(3) universality class.

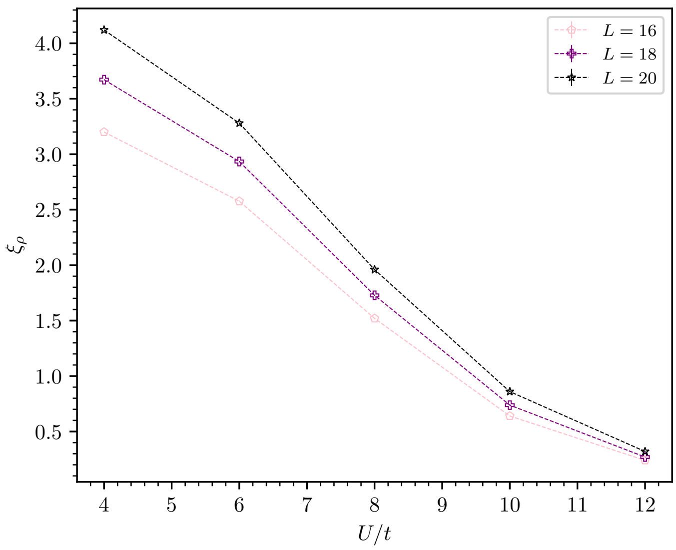

FIG. R1: The relationship between ξ_ρ and U/t in DQMC-finite-T of the Hubbard model on a cubic lattice near the critical temperature when $L = 16, 18$ and 20.

Summary of changes to manuscript

According to the respected referees' comments, we made the following revisions.

- We make our contribution in the abstract and introduction clearer.
- We have added reference Phys. Rev. B 99, 125145 (2019).
- We have added the appendix G to explain the universality class and finite-size effects of the model.
- Some typos are fixed.