

Dear Editors,

we thank the referees for their helpful reports, and apologize for the lengthy “awaiting resubmission” status of our manuscript on the SciPost submission web site. We have finally revised the manuscript heeding the advice of the two referees.

We reply to their suggestions, questions, and criticism below. The referee reports are *italicized* and our replies are non-italicized.

Reply to Report of the 1st Referee

Strengths

- 1 - The problem of time dynamics in quantum many-body systems is challenging as there are no general well-developed tools for addressing it while experimentally such dynamics can be studied. In that context, a time-dependent version of HNC method provides a useful numerical method of addressing time-dependent problems in a non-perturbative way
- 2 - The tHNC method is verified in 1D and 2D geometry in comparison to tVMC predictions. There is a good agreement for the first few oscillations after the quench.

Weaknesses

- 1 The structure of the article can be improved. It would be more natural to present first the methodology, then the verification (1D and 2D), and leave the new results (3D) for the last.
- 2 There are some unnecessary technical details given while the physical motivation is missing.

Report

Authors study the problem of finding the time dependence in a quantum many-body system which is on its own very interesting and difficult task, as there are no standard and well-established techniques for doing so numerically. A method based on hypernetted-chain approach is developed and applied to the problem of interaction quenches in one, two, and three dimensions. While the developed method is interesting I believe presentation can be significantly improved.

Requested changes

Main comments:

- 1 The way the article is structured now, first 3D results are shown and later verification of the method is done in 1D and 2D. It feels more natural to show first verification of the method and later apply it to some system where no alternative results are present.

We agree that it is common to start with simpler cases for verification of a method. But there is a reason that we first present the main results for 3D: one important message is that the creation of roton pairs lead to persistent oscillations in $g(r, t)$ for small r . We see the same effect in 1D and 2D, but if we had started with the 1D and 2D verification results, we either have to defer to the later tHNC results in 3D where we study the effect systematically for many quench strengths; or we have to explain them already for 1D and 2D which takes away the spotlight from the main results obtained for 3D. Therefore we prefer to lead with the main results.

- 2 Is it possible to predict the error of the obtained results within the used theory? It might be anticipated that the error is larger for larger times. Is it possible to see that?

The simplest check is energy conservation after the quench. Due to numerics we usually see a light increase of the energy, which can be reduced by using a smaller time step. We are not aware of a general symplectic method for nonlinear partial integro-differential equations, but this is an interesting technical question on which we have been working on. The positive message is that despite the approximations of tHNC, energy is conserved apart from time step errors.

Nonetheless the comparison with tVMC shows that $g(r, t)$ is affected by these approximation, since both tHNC and tVMC use the same Jastrow ansatz but start to deviate particularly for large t and small r (see Fig.8).

Within the tHNC theory, the error could be studied by: (i) replacing the superposition approximation for g_3 with another approximation such as convolution approximation – we tried this but the resulting equation turned out to be numerically less stable (as mentioned above, improving the numerical integration of the

tHNC equations is an important task). (ii) including a better approximation to the so-called elementary diagrams in the HNC equation (6) instead of completely neglecting them – this is probably possible without numerical complications and without making the computations much slower (the efficiency of tHNC compared to tVMC is its selling point), but we have not done this for this first presentation of our new method. It's certainly high in the to-do list. (iii) including triplet correlations which has been done for ground state and linear response calculations. This is a project for the far future, since we expect this to become very complicated without a genuinely new approach to solve the resulting high-dimensional equations of motions.

We mentioned these improvements in section 4, and further extended this discussion in the revision.

3 In the benchmark tests, tHNC results are compared to predictions of tVMC method (for example Fig. 8). For small times there is a good agreement, for larger times differences are visible. Is it possible to add error bars to both theories to make the comparison quantitative?

Your question prompted us to perform additional tVMC simulations to get a better idea of the stochastic error of $g(r, t)$. In the revision we add error bounds in Fig.7. The effect of stochastic noise increases over time, which is intuitively clear because in every time step of the propagation, we perform a variational Monte Carlo calculation which is bound to add noise. Note that the result incorporating the additional tVMC simulations does not exhibit an apparent increase of the oscillation amplitude of $g(r, t)$.

We did not include the error bound in Fig. 5 and 6, where we show $g(r, t)$ for all r , since this would render the figures unintelligible. We observed that the increase of the statistical error with time is true for all r .

In the manuscript we extended the description of the results by mentioning the statistical error of tVMC.

The other, more fundamental source of error are the approximations such as restricting ourselves to pair correlations $u_2(r, t)$. We cannot give this systematic error because the exact $g(r, t)$ is not known. In particular, we cannot give an error for tHNC because we cannot quantify the effect of the approximations incorporated into the tHNC equation (10). This leads us back to your question 2 about predicting the error.

4 Comment why the imaginary part of $u_2(r) = u(r) + 2i\phi(r)$ has a factor of two as compared to the real part

There is no physical reason that we choose this convention: in the literature for the HNC-EL method, u has a factor $\frac{1}{2}$ in the Jastrow ansatz because it becomes 1 in $|\Phi_0|^2$, leading a factor 1 in the HNC equation (6). The imaginary part does not appear in $|\Phi_0|^2$, and thus not in the HNC equation. Therefore we decided to do without the factor $\frac{1}{2}$ for $\phi(r)$ in the Jastrow ansatz.

5 When energy is given in units of E_0 , it is not clear if energy per particle or defect energy is assumed.

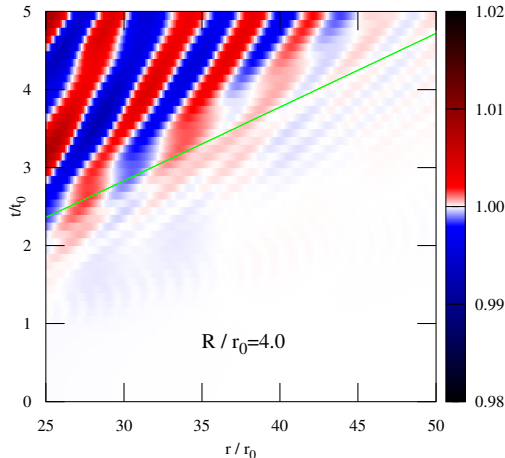
We always mean energy per particle, where the energy is the total energy, i.e. not the energy measured from the ground state energy.

6 Below Fig. 1, pair distribution is given for different values of R/r_0 . It might be useful as well to report the smallest and the largest corresponding density, i.e. ρr_0^3 .

We use the average neighbor distance as length unit r_0 (apart from the Fermi-inspired prefactor in 3D and 2D). Therefore in our units the density is always the same: $\rho r_0^3 = (6\pi^2)^{-1}$ in 3D, $\rho r_0^2 = (4\pi)^{-1}$ in 2D, and $\rho r_0 = 1$ in 1D. We add a bracket in the 1st paragraph of section 3.1 stating this.

7 Fig. 2, it is commented that no light cone boundary is observed. Still, the actual boundary looks pretty linear for practical purposes. It might be useful to draw the light cone defined by the speed of sound in the bulk with a dashed line for comparison.

We follow up on this suggestion, and added a light-cone in Fig.2, based on the speed of sound c , i.e. it is actually a sound cone. In the pair distribution it is shown as a line $r = 2ct$, which we superimpose on the maps of $g(r, t)$ in Fig.2. For smaller R_1 the sound cone is not at all a boundary for the evolution of $g(r, t)$ because in this case many excitation with higher group velocity v_g than the sound velocity c are excited.



For larger R_1 , the sound cone appears to be a boundary, but a closer look shows there are always oscillations of small amplitude but high wave number that are faster than the sound cone limit – in the included figure we show $g(r, t)$ for $R_1/r_0 = 4.0$ on a zoomed color scale, together with the sound cone (green line). We did not add an extra figure to demonstrate this, because the “light cone” is not a the focus of this paper. But we added an extensive explanation and discussion of the sound cones shown now in Fig.2.

8 Fig. 2, color coding (blue-red) is not explained.

We added a color bar to Fig.2, with an explanation in the caption.

9 “The effect of non-linearity is demonstrated ...”. Please provide a more detailed explanation of what is meant by a linear / nonlinear effect.

We did not explain this very well, because the other referee had in fact the same question. Please refer to our answer to question 3 of the other referee.

We added a corresponding explanation in the text.

10 Sections on 1D and 2D comparison provide technical details which can be moved to the appendix. Instead, it would be good to state the physical motivation which systems are considered and why.

We follow the suggestion of the referee and moved the technical details to the appendix.

Minor comments

11 Visually it does not look nice to start a phrase with a lowercase letter (“tHNC ...”) or symbols (“L...”, “g(r,t)”, “g”, “g₃”, “w_I”, “β”, “γ”, etc) . Please rephrase.

The corresponding sentences have been rephrased.

12 “We do not include an external potential because we only consider homogeneous systems” Explain better the reasoning as right now it is tautologic.

We expanded and rephrased this paragraph.

13 "In the case that the perturbation is a change of perturbation, the only difference .. is the time-dependence of perturbation". Tautology once again.

We rephrased this sentence.

14 "Note that γ in eq.(10) is to be calculated from its gradient" Rephrase

We rephrased the sentence.

15 "When two particles are closer than ... they are only weakly repelled because u becomes flat", explain the physical reason (Rydberg blockade?) rather than the mathematical property of the used model

The physical reason is coupling of the atomic ground state and a Rydberg state with a laser detuned from resonance. Roughly speaking this couples the two potential energy surfaces of two atoms (ground-ground and Rydberg-Rydberg) which can be described approximately by an effective interaction. The $1/r^6$ part comes from the Rydberg state and the flat part from the atom state (where the particles do not feel an interaction on the range of R).

This is described in the early papers on Rydberg-dressed atoms, so we do not provide a derivation. At the start of section 3.1, we added this physical picture with references (including a new one, Pupillo et al, PRL 104, 223002 (2010)) that derive this effective interaction.

16 "For the 1D comparison we use a square well potential", just saying "potential" might be ambiguous as applied to external potential or interaction potential.

We rephrased this to make clear we use a square well *interaction* potential.

17 "We approximate the Jastrow pair-correlation ... with 400 splines". Is it a single spline function containing 400 parameters or are there 400 spline functions?

We use a cubic spline function with 400 complex valued weights, corresponding to 400 time-dependent parameters. We rephrased and moved this part to the appendix.

18 For some reason Fermi units are used in 2D and 3D but not in 1D, although this is a matter of choice and can be left as it is.

Although we understand the point raised by the referee, we decided to leave the units as they are in the initial submission because we used it already in a previous publication on Rydberg-dressed Bose gases (Seydi et al, Ref.[36] in the old manuscript).

List of Changes:

1. We added a comparison of the computational effort of tHNC and tVMC.
2. We explain what we mean by “nonlinear process”
3. We provide a comparison between the Bogoliubov approximation, the HNC approximation and the exact result for $g(r)$ in the ground state in a new appendix C, including a new Fig.8.
4. We improved Fig.2 and its caption: adding a color bar, adding the sound cone and explaining the color scheme;
5. At the start of the results sections we elaborated a bit more on how the result section is structured
6. At the start of section 3.1 we give a physical picture of the Rydberg-dressed interaction.
7. We moved the technical details of the tVMC simulations to the appendix.
8. We extended the discussion of the “light cone” ideas considerably, describing and explaining the additional light cone lines in Fig.1.
9. We combined former Fig.1 and 4 into one Fig. with two panels, because in the new discussion of the light cone we need to refer to Fig.4 earlier in the text than in the old manuscript.
10. We updated Fig.7 (former Fig.8) by showing the stochastic error.
11. We converted the inline equation for the action S into equation (4) in order to reference this definition in app.A
12. In app. A, we explicitly show the time dependence of all quantities instead of omitting it
13. We added a reference for Feshbach resonances in the introduction
14. various small changes in formulation

New References:

1. A. Kerman and S. Koonin, *Annals of Physics* 100, 332–358 (1976).
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5. L. Madeira and V. S. Bagnato, *Symm.* 14, 678 (2022)
6. F. Dalfovo, S. Giorgini, L. P. Pitaevskii and S. Stringari, *Rev. Mod. Phys.* 71, 463 (1999)
7. O. Morsch and M. Oberthaler, *Rev. Mod. Phys.* 78, 179 (2006).
8. A. Polkovnikov et al., *Rev. Mod. Phys.* 83, 863 (2011)
9. T. Langen, R. Geiger and J. Schmiedmayer, *Annu. Rev. Condens. Matter Phys.* 6, 201 (2015)
10. M. Cheneau et al., *Nature* 481, 484 (2012)
11. P. Makotyn, *Nat. Phys.* 10, 116(2014)
12. N. Navon et al.,*Nat. Phys.* 17(12), 1334 (2021)