

Thesis Changes Log

Name of Candidate: Andrei E. Tarkhov

PhD Program: Physics

Title of Thesis: Ergodization dynamics of the Gross-Pitaevskii equation on a lattice

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Chair of PhD defense Jury: Prof. Nikolay Gippius

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Date of Thesis Defense: 23 October 2020

The thesis document includes the following changes in answer to the external review process.

Dear Jury Members,

we would like to thank you for your time and effort to assess the manuscript of my Thesis. Your comments and critique helped significantly improve the quality and coherence of the manuscript. We really appreciate your reviews.

Below, we address all the critical comments and suggestions one by one.

Reviewer: Prof. Sergej Flach

1. P.22: Section 1.4. discusses microcanonical thermodynamics and the way to microcanonically measure temperature. Since the GP system also conserves the norm, the chemical potential is another relevant parameter. How can that quantity be measured? How are the relations (1.9) and (1.10) taking the existence of the chemical potential into account?

The chemical potential can be also extracted from the same sampling procedure. The chemical potential was not necessary for the purposes of the Thesis, hence the procedure for its calculation was omitted. Now, we added relation for calculation of the chemical potential from the sampling of the vicinity of a phase space point in the end of Section 1.4, see new Eq. (1.12), which is a counterpart of former equation (1.10) for temperature.

2. P.26 2nd paragraph: ‘above $\beta=0$ ’ is not a clear. Since β is a real number, above zero would mean positive temperatures. But that is not what the author probably had in mind.

Indeed, we had in mind that in microcanonical simulations one can choose a microcanonical state with energy higher than the one corresponding to $\beta=0$. Thus, we corrected this phrase in the text to “In the last two decades, the non-Gibbs states at energies higher than those corresponding to $\beta=0$ have been extensively studied.”

3. P.26 2nd paragraph: ‘astronomically large ... times’ is not a scientifically sound statement.

We corrected the phrase to “such states for 1D DGPE chains, may equilibrate at times inaccessible in numerical simulations”.

4. P.32 below (2.1): what defines the transient regime time length?

The transient regime length is defined as the time when the largest Lyapunov exponent is not dominant yet, and all Lyapunov exponents contribute to the growth.

5. P.34: ‘fixed such that $\epsilon=1$...’ – ϵ seems not to be defined. What is that? The energy density? And what is then the corresponding inverse temperature β ? I guessed it is infinite, implying the simulations are done on the borderline between Gibbs and nonGibbs dynamics?

ϵ is the energy per lattice site. The corresponding inverse microcanonical temperature is 2...6 dependent on the dimensionality of the lattice. The following correction added to the text: “fixed such that the energy per one site $\epsilon=1$ (corresponding to the microcanonical temperature $T \sim 2 \dots 6$ dependent on the dimensionality of the lattice), see Eq.~(\ref{Intro:eq:energy_density_def})...”

6. P.35 section 2.3: why did the author choose RK? Why not some symplectic algorithm? At least a few words on the reasons for that choice of the integrator would be appropriate.

The correction to the text added: “The choice of a relatively simple integrator (Runge-Kutta) is justified by the fact that the energy drift of the DGPE solutions due to the non-symplectic nature of the algorithm is negligible for the purposes of this Thesis. See Ref~\cite{danieli2018computational} for more advanced integration schemes.” The paper discussing more advanced integrators, including symplectic ones, is now cited.

7. P.36 section 2.3.1: Am I correct in assuming that the slightly perturbed trajectory was integrated using the full nonlinear GP generated differential equations? If so, why did the author not implement the usual method of tangent dynamics and variational equations?

Since, the focus of the Thesis is on the largest Lyapunov exponent, and not on the full Lyapunov spectrum, the integration of DGPE equations for two initial conditions turns out computationally easier than solving tangent dynamics and variational equations. Computational memory limitations are especially challenging for large systems, e.g. 3D lattices $50 \times 50 \times 50$, since the memory for storing the Hessian matrix grows quadratically with the system size $(2V)^2$.

8. Chapter 3: there are plenty of other ergodization time scales defined in the literature. I am missing a discussion and comparison with the one used in this thesis.

In the beginning of Chapter 3, we added a discussion of another method of estimating an ergodization time “The ergodization time can be also defined as a typical self-averaging time for a chosen observable~\cite{mithun2019dynamical}, however, such a definition depends on the choice of the observable, which, in turn, make it difficult to compare ergodization times in systems with qualitatively different degrees of freedom.”

9. P.45: ‘sufficiently long’ is not clear.

We replaced it with: “The largest Lyapunov exponent can be calculated as the average of instantaneous stretching rates over time...”.

10. P.45: ‘dynamically localized’ is not clear.

We added:

“The Lyapunov eigenvectors are normally localized in the sense that the projections on the axes representing individual sites are large only for a small subset of sites, which itself depends on time t .”

11. P.77 section 4.7: Nice result! But why does the largest LE does not indicate the slowing down at the phase transition? And isn’t that result precisely a case where the LE based ergodization time fails to predict the true ergodization times? If so, then when does do the right work?

The LE is sensitive to the fastest dynamics of the system at a few sites (comprising the projection of the Lyapunov eigenvector), whereas the slowing down due to the crossing a second order phase transition rather occurs at slower timescales and larger spatial scales. For this reason, the LE is insensitive to the phase transition. Hence, the ergodization time defined from the Lyapunov process is also insensitive to the phase transition.

We added a remark in the end of Section 4.7. “This finding is consistent with the remark made in Section~\ref{pap2:sec:def_of_erg_time_from_LE} that the ergodization time characterizes the dynamics of the system on the spatial scale of a few lattice sites. Thus, it is not sensitive to the very slow relaxation of large-scale topological objects.”

Reviewer: Prof. Anton Andreev

My only comment is that I am skeptical about the relevance of the studies of quenches in DGPT to the experiments on laser-induced CDW melting. Optical excitations produce electronic excitations with energies of order eV, which greatly exceed the CDW energy scale. By cascading down in energy, these initial excitations create multiple low energy quasiparticles, which are very likely to be important in the subsequent dynamics of the CDW order parameter. The quench dynamics of the DGPT model lacks such excitations and describes purely Hamiltonian dynamics. In contrast, the dynamics of the CDW order parameter should to be dissipative due to coupling to quasiparticle excitations. However, in my opinion the detailed discussion of the mapping of DCW dynamics onto DGPT is a stretch.

It was not clearly stated in the manuscript that there was another published work “Pavel E Dolgirev et al. “Amplitude dynamics of the charge density wave in LaTe3: Theoretical description of pump-probe experiments”. *Physical Review B* **101.5** (2020), p. 054203.”, which focused on the concerns of the reviewers. Specifically, the findings of the paper show that indeed initially the electronic subsystem absorbs almost all energy of the laser pulse, and its order parameter is different from the order parameter of the lattice. However, after a quick relaxation process taking of order of 2 ps, the electronic subsystem dissipates its energy into the lattice (so-called “hot phonons”), and effectively the system can be described by a single CDW order parameter (for both the lattice and the electronic subsystems, since they are tightly correlated after 2 ps). Hence, the detailed discussion of the mapping of CDW dynamics onto DGPE is considered applicable only after the initial relaxation has finished, and the system can be described by a single order parameter. The dissipation due to coupling to electron quasiparticle excitations is sufficiently small because of the relatively small specific heat of the electronic subsystem. Thus, we argue that the purely Hamiltonian dynamics of DGPE is a reasonable approximation to the true CDW dynamics after 2 ps.

We added a paragraph in the end of Section 4.1 “The findings of Ref.~\cite{dolgirev2020amplitude} indicate that the initial response of LaTe₃ following a strong photoexcitation is not describable by a single order parameter because the energy of the laser pulse is mainly absorbed by the electronic subsystem and then it takes a time about 2 ps for the electronic subsystem to dissipate its energy into the lattice. Only after that, the local behavior of the system can be described by a single CDW order parameter. It is the relaxation in this later-time regime that we would like to describe with the help of the DGPE. The question can still arise whether the calculations based on the purely Hamiltonian DGPE dynamics would miss the dissipative contribution due to the coupling to the electronic excitations. Such a contribution certainly exists in the real material. However, we assume that, due to the smallness of the electronic specific heat relative to that of the lattice, the dissipation caused by the electronic excitations is sufficiently small to justify the applicability of the DGPE-based quench simulations for times longer than 2 ps.”

Reviewer: Associate Prof. Astrid de Wijn

The final chapter, chapter 5, is supposed to link the previous chapters together, and back to the thesis topic, but is lacking in this regard. It is now just a summary. It would have been interesting to see the candidate’s ideas on the usefulness for example of his ergodization time for the experimental setting of chapter 4, and in a broader context. I find the ergodization time an interesting concept, but I am left with questions on both its relevance for non-equilibrium systems and relation to the mathematical

concept of ergodicity. In my opinion this thesis contains sufficient new material to meet the international standards for defense. To improve the thesis further, I do recommend that the candidate expands on the discussion in chapter 5.

We added a paragraph to Chapter 5: “Overall, the ergodization process in a many-particle system cannot be characterized by a single timescale. The findings of this Thesis support the view that the ergodization dynamics of many-particle systems is hierarchical in terms of timescales. At faster timescales, the Lyapunov process is dominant: it can be used to quantify the ergodization timescale relevant to establishing the local quasi-equilibrium. Our findings further indicate that on very long timescales, the appearance and disappearance of large topological objects are one of the factors determining the approach to the true equilibrium.”

Reviewers: Prof. N. Berloff, Prof. P. Lagoudakis, Prof. N. Gippius

No questions or suggestions to address.