LIEB–ROBINSON BOUNDS AND THE EXISTENCE OF INFINITE SYSTEM DYNAMICS

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We present a recent result on the existence of the dynamics in the thermodynamic limit of a class of anharmonic quantum oscillator lattices, which was obtained using Lieb–Robinson bounds.

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1. Introduction

In condensed matter physics, three common types of degrees of freedom are often found together: atoms positioned in a lattice, spin magnetic moments, and itinerant electrons. Many phenomena primarily involve only one of these and it has therefore proved useful to study them with separate models. Here, we are concerned with the spatial degrees of freedom of atoms in a lattice. The fact that the atoms oscillate about their equilibrium positions is essential for many important phenomena in condensed matter physics. The question we address is whether one can define the time evolution, consistent with the Schrödinger equation, for an infinite assembly of quantum oscillators such as a crystal lattice.

It is natural to start by considering the standard harmonic interaction, which should be an accurate description when the displacements from the equilibrium positions are small. It is well known, however, that some basic phenomena require that we consider anharmonic perturbations. Our approach applies to multi-body interactions that fall off sufficiently fast but for clarity and space limitations we will restrict ourselves to local and nearest neighbor anharmonicities here and refer to our forthcoming paper for the general case. We will also limit the discussion to oscillators organized in a translation-invariant fashion on a lattice. To keep the notation simple we will work with one-dimensional oscillators at each lattice site, but this is not essential. With some straightforward modifications of the analysis our main result can be generalized to non-translation invariant models defined on a graph satisfying a few natural assumptions.
2. Harmonic lattice systems

Let \( \Lambda \) denote a finite subset of the \( \nu \)-dimensional hypercubic lattice \( \mathbb{Z}^\nu \) and define Hamiltonians \( H_\Lambda \) as self-adjoint operators on \( \mathcal{H}_\Lambda = \bigotimes_{x \in \Lambda} L^2(\mathbb{R}) \) by the following expression

\[
H_\Lambda = \sum_{x \in \Lambda} \frac{1}{2m} p_x^2 + \frac{m}{2} \omega^2 q_x^2 + V(q_x) + \sum_{x, y \in \Lambda, |x - y| = 1} \lambda(q_x - q_y)^2 + \Phi(q_x - q_y)
\]

where \( \omega, \lambda, \geq 0 \), and \( p_x \) and \( q_x \) are the canonical momentum and position operators for the oscillator at \( x \in \Lambda \). The Heisenberg dynamics, \( \{ \tau^{\Lambda}_t \}_{t \in \mathbb{R}} \), is defined by

\[
\tau^{\Lambda}_t(A) = e^{itH_\Lambda} A e^{-itH_\Lambda}, \quad A \in \mathcal{B}(\mathcal{H}_\Lambda).
\]

The algebra of observables is a tensor product

\[
\mathcal{B}(\mathcal{H}_\Lambda) = \bigotimes_{x \in \Lambda} \mathcal{B}(\mathcal{H}_x) \equiv \mathcal{A}_\Lambda
\]

such that for \( X \subset \Lambda \), we have \( \mathcal{A}_X \subset \mathcal{A}_\Lambda \), by identifying \( A \in \mathcal{A}_X \) with \( A \otimes I_{\Lambda \setminus X} \in \mathcal{A}_\Lambda \).

Our main concern is the existence of a limiting dynamics: do we have \( \tau_t \) such that

\[
\tau^{\Lambda}_t(A) \longrightarrow \tau_t(A), \quad \text{as } \Lambda \uparrow \mathbb{Z}^\nu
\]

in a suitable sense? For an anharmonic lattice of classical oscillators a positive answer to this question was obtained by Lanford, Lebowitz and Lieb.\(^4\)

It is well-known that in the case of quantum spin systems (i.e., bounded local Hamiltonians) one can use Lieb-Robinson bounds to establish the existence of the thermodynamic limit.\(^2\) The essential observation is as follows. Let \( \Lambda_n \) be an increasing exhausting sequence of finite volumes with Hamiltonians of the form

\[
H_{\Lambda_n} = \sum_{X \subset \Lambda_n} \Phi(X)
\]

where \( \Phi(X) = \Phi(X)^* \in \mathcal{A}_X \). Then, for \( n > m \), one easily derives the bound:

\[
\| \tau^{\Lambda_n}_t(A) - \tau^{\Lambda_m}_t(A) \| \leq \sum_{x \in \Lambda_n \setminus \Lambda_m} \sum_{X \ni x} \int_0^{|t|} \| [\Phi(X), \tau^{\Lambda_m}_s(A)] \| \, ds. \quad (1)
\]

Therefore, if we can show that the commutators in the integrand have sufficiently small norms, it will follow that the finite-volume dynamics form a Cauchy sequence. Estimates for such commutators were first derived by Lieb and Robinson.\(^5\) For \( A \in \mathcal{A}_X \) and \( B \in \mathcal{A}_Y \), they proved a bound of the form

\[
\| [\tau_t(A), B] \| \leq C e^{-at(d(X,Y) - v|t|)},
\]

where \( C, a, \) and \( v \) are positive constants and \( d(X,Y) \) denotes the distance between \( X \) and \( Y \). Estimates of this type are now commonly referred to as Lieb-Robinson bounds.\(^3,7-9\) For anharmonic lattice systems Lieb-Robinson bounds were recently proved in Ref. 10, and this work builds on the results obtained there.
For the oscillator lattices with $\lambda \neq 0$, the approach suggested by Eq. 1 does not work due to the unboundedness of $(q_x - q_y)^2$. But we note that for the harmonic lattice, $\tau^\Lambda_t$ can be calculated explicitly and can also be defined for the infinite lattice. One then sees, however, that $\tau^\Lambda_t(A)$ cannot converge in norm. The idea is to consider the infinite anharmonic system as a limit of finite-volume perturbations of the infinite harmonic system. We mention that, with a different approach, Amour, Levy-Bruhl, and Nourrigat have recently obtained convergence results for certain models by introducing suitable Sobolev-like norms for the observables.\

Rigorous perturbation theory of infinite systems is available if the unperturbed infinite system dynamics has a suitable continuity property. In our case this will be continuity for the weak operator topology, which follows from known properties and the exact solution of the harmonic lattice.

Up to a redefinition of the parameters, the harmonic lattice model Hamiltonian on a finite subset $\Lambda \subset \mathbb{Z}^\nu$, is

$$H_\Lambda = \sum_{x \in \Lambda} p_x^2 + \omega^2 q_x^2 + \sum_{|x-y|=1} \lambda (q_x - q_y)^2$$

acting on $\mathcal{H}_\Lambda$. The creation and annihilation operators are defined by

$$a_x = \frac{1}{\sqrt{2}} (q_x + ip_x) \quad \text{and} \quad a_x^* = \frac{1}{\sqrt{2}} (q_x - ip_x),$$

which satisfy the Canonical Commutation Relations (CCR):

$$[a_x, a_y] = [a_x^*, a_y^*] = 0 \quad \text{and} \quad [a_x, a_y^*] = \delta_{x,y} \quad \text{for all} \ x, y \in \Lambda_L$$

$H_\Lambda$ is a quadratic expression in $a_x, a_x^*$, which can be diagonalized by a Bogoliubov transformation. This is usually done in Fourier space resulting in:

$$H_\Lambda = \sum_{k \in \Lambda^*} \gamma(k) (2b_k^* b_k + 1)$$

where $\gamma(k) = (\omega^2 + 4\lambda \sum_{j=1}^{\nu} \sin^2(k_j/2))^{1/2}$. The $b_k^*$ are creation operators for the eigenmodes of the system, which also satisfy the CCR, and the ground state of $H_\Lambda$ is the corresponding vacuum. The time evolution is simply given by $\tau_t(b_k^*) = e^{-2\gamma(k)t}b_k^*$. It is useful for us to express the Bogoliubov transformations in real space: for each $f : \Lambda_L \to \mathbb{C}$, set

$$a(f) = \sum_{x \in \Lambda_L} f(x)^* a_x, \quad a^*(f) = \sum_{x \in \Lambda_L} f(x) a_x^*.$$ 

and similarly for the $b$'s. Then, there are real-linear operators $U$ and $V$ such that

$$a(f) = b(U^* f) - b^*(V^* f), \quad a^*(f) = b^*(U^* f) - b^*(V^* f).$$

Using these relations, one finds a one-parameter group, $T_t$, such that

$$\tau_t(a(f)) = \tau_t(b(U^* f) - b^*(V^* f)) = a(T_t f), \quad \tau_t(a^*(f)) = a^*(T_t f).$$
Since the canonical operators (p’s, q’s, a’s, a*’s,...) are all unbounded, we will derive Lieb-Robinson bounds for the Weyl operators instead:

\[ W(f) = \exp \left[ \frac{i}{\sqrt{2}} (a(f) + a^*(f)) \right] , \]

This can be done very explicitly by using the relations

\[ \tau_t(W(f)) = W(T_t f) , \quad \text{and} \quad W(f)W(g) = e^{i\sigma(f,g)}W(f + g) \]

where \( \sigma(f,g) = \text{Im}(f,g) \). Observe that

\[ [\tau_t(W(f)), W(g)] = \{W(T_t f) - W(g)W(T_t f)W(-g)\} W(g) \]

\[ = \left\{ 1 - e^{-2i\sigma(T_t f,g)} \right\} W(T_t f)W(g) . \]

Since the Weyl operators are unitary, we therefore have \( \| \tau_t(W(f)), W(g)\| \leq 2|\sigma(T_t f,g)| \). So, all we have to do is to estimate \( \sigma(T_t f, g) \). \( T_t f \) is explicitly given by

\[ T_t f = f \ast h_{1,t}^{(L)} \ast \overline{f} \ast h_{2,t}^{(L)} , \]

where the functions \( h_{1,t} \) and \( h_{2,t} \) are given by

\[ h_{1,t}^{(L)}(x) = \frac{i}{2} \text{Im} \left[ \frac{1}{|\Lambda_L|} \sum_{k \in \Lambda_L} (\gamma(k) + \gamma(k)^{-1}) e^{ikx - 2i\gamma(k)t} \right] + \text{Re} \left[ \frac{1}{|\Lambda_L|} \sum_{k \in \Lambda_L} e^{ikx - 2i\gamma(k)t} \right] \]

\[ h_{2,t}^{(L)}(x) = \frac{i}{2} \text{Im} \left[ \frac{1}{|\Lambda_L|} \sum_{k \in \Lambda_L} (\gamma(k) - \gamma(k)^{-1}) e^{ikx - 2i\gamma(k)t} \right] . \]

By analyzing these functions one then shows that for every \( a > 0 \), there exist \( c_a \) and \( v_a \) such that

\[ |\sigma(T_t f, g)| \leq c_a e^{v_a |t|} \sum_{x,y} |f(x)||g(y)| e^{-a d(x,y)} . \]

**Theorem 2.1 (Ref. 10).** Let \( \lambda, \omega \geq 0 \). Then, for all \( f, g \) with \( \text{supp} f \subset X \) and \( \text{supp} g \subset Y \),

\[ \| [\tau_t(W(f)), W(g)] \| \leq C \sum_{x,y} |f(x)||g(y)| e^{-2d(x,y) - v |t|} , \]

with \( v = 6\sqrt{\omega^2 + 4\nu\lambda} \).

### 3. Anharmonic lattice systems

In Ref. 10 we proved Lieb-Robinson bounds for finite systems, with estimates uniform in the volume. With the same approach one can also prove bounds for harmonic infinite systems with an anharmonic perturbation in finite volume, i.e., a model with formal Hamiltonian of the form:

\[ H_\Lambda = \sum_{x \in \mathbb{Z}^d} p_x^2 + \omega_x^2 q_x^2 + \sum_{x,y \in \mathbb{Z}^d, |x-y|=1} \lambda(q_x - q_y)^2 + \sum_{X \subset \Lambda} \Phi(X) . \]

Typical \( \Phi \) are \( \Phi(\{x\}) = V(q_x) \), \( \Phi(\{x, y\}) = W(q_x - q_y) \), etc. but more general perturbations can be considered.\( ^11 \)
For the harmonic system, we can directly see how the exact expressions extend to the infinite system. For \( f : \mathbb{Z}^\nu \rightarrow \mathbb{C} \) in a suitable function space (\( \ell^1(\mathbb{Z}^\nu) \), or \( \ell^2(\mathbb{Z}^\nu) \)), it is straightforward to define

\[
\tau_t(W(f)) = W(T_t f)
\]

We get a Hilbert space representation by representing the Weyl operators on the Fock space generated by the \( b^*(f) \) operators acting on the vacuum. On this space we have well-defined Hamiltonian such that

\[
\tau_t(W(f)) = e^{itH}W(f)e^{-itH}
\]

\( \tau_t \) is the dynamics for the formal Hamiltonian

\[
H = \sum_{x \in \mathbb{Z}^\nu} p_x^2 + \omega^2 q_x^2 + \sum_{|x-y|=1} \lambda(q_x - q_y)^2
\]

and the Lieb-Robinson bounds continue to hold.

For simplicity, consider the perturbation of the form \( P_\lambda = \sum_{x \in \Lambda} V(q_x) \). Then, the perturbed dynamics, formally corresponding to \( H + P_\lambda \), and can be defined mathematically by the Dyson series:

\[
\tau_t^{(\lambda)}(W(f)) = \tau_t(W(f)) + \sum_{n=1}^\infty i^n \int_{0 \leq t_1 \leq t_2 \leq \cdots \leq t} dt_1 \cdots dt_n [\tau_{t_n}(P_\lambda), \cdots [\tau_{t_1}(P_\lambda), \tau_t(W(f))]]
\]

We have the following Lieb-Robinson bounds for \( \tau_t^{(\lambda)} \).

**Theorem 3.1 (Ref. 10).** Let \( \lambda \geq 0, \omega > 0, \) and \( V \) such that \( \|k^2 \hat{V}(k)\|_1 < \infty \). Then, for all \( f, g \in \ell^1(\mathbb{Z}^\nu) \), we have

\[
\left\| \left[ \tau_t^{(\lambda)}(W(f)), W(g) \right] \right\| \leq C \sum_{x \neq y} |f(x)||g(y)|e^{-2(d(x,y) - v|t|)}
\]

with

\[
v = 6 \sqrt{\omega^2 + 4\nu \lambda} + c\|k^2 \hat{V}(k)\|_1.
\]

To show convergence, we estimate \( \|\tau_t^{\Lambda_n}(W(f)) - \tau_t^{\Lambda_m}(W(f))\| \), for \( \Lambda_m \subset \Lambda_n \) by considering \( \tau_t^{\Lambda_m} \) as a perturbation of \( \tau_t^{\Lambda_n} \). This gives

\[
\tau_t^{\Lambda_n}(W(f)) = \tau_t^{\Lambda_n}(W(f)) + i \int_0^t \tau_s^{\Lambda_n} \left( \left[ P_{\Lambda_n \backslash \Lambda_m}, \tau_t^{\Lambda_m}(W(f)) \right] \right) ds,
\]

Therefore

\[
\left\| \tau_t^{\Lambda_n}(W(f)) - \tau_t^{\Lambda_m}(W(f)) \right\| \leq \sum_{z \in \Lambda_n \backslash \Lambda_m} \int_0^{|t|} \left\| \left[ V(q_z), \tau_{t-s}^{\Lambda_m}(W(f)) \right] \right\| ds
\]

By writing \( V(q_x) = \int \hat{V}(p) W(p\delta_x) dp \), \( W(p\delta_x) = e^{ipq_x} \), we can then use Theorem 3.11 for \( \tau_t^{\Lambda_m} \) to obtain the convergence. The convergence is uniform on intervals \([-t_0, t_0] \). We also immediately get continuity in \( t \) of the limiting dynamics by an \( \epsilon/3 \) argument.
**Theorem 3.2 (Ref. 11).** Assume $\omega > 0$, $\| k\hat{V}(k) \|_1 < \infty$, $\| k^2 \hat{V}(k) \|_1 < \infty$. For all $f \in \ell^1(\mathbb{Z}^n)$, and all $t \in \mathbb{R}$, the limit
\[
\lim_{\Lambda \uparrow \mathbb{Z}^n} \tau^\Lambda_t(W(f)) = \tau^\infty_t(W(f))
\]
converges in the operator norm topology and the resulting the dynamics is continuous in $t$ in the weak operator topology.

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**References**

1. L. Amour, P. Levy-Bruhl, and J. Nourrigat, *Dynamics and Lieb-Robinson Estimates for Lattices of Interacting Anharmonic Oscillators*. [arXiv:0904.2717](http://arxiv.org/abs/0904.2717).
2. O. Brattelli and D. W. Robinson, *Operator Algebras and Quantum Statistical Mechanics. Volume 2.*, 2nd Edition (Springer-Verlag, 1997).
3. M. Hastings and T. Koma, Commun. Math. Phys. 265, 781–804 (2006).
4. O.E. Lanford, J. Lebowitz, E. H. Lieb, J. Statist. Phys. 16, 453–461 (1977).
5. E.H. Lieb and D.W. Robinson, Comm. Math. Phys. 28, 251–257 (1972).
6. J. Manuceau and A. Verbeure, Commun. Math. Phys. 9, 293–302 (1968).
7. B. Nachtergaele and R. Sims, Commun. Math. Phys. 265, 119–130 (2006).
8. B. Nachtergaele, Y. Ogata, and R. Sims, J. Stat. Phys. 124, 1–13 (2006).
9. B. Nachtergaele and R. Sims. *Locality Estimates for Quantum Spin Systems*. To appear in: Sidoravicius, Vladas (Ed.), *New Trends in Mathematical Physics. Selected contributions of the XVth International Congress on Mathematical Physics*, Springer Verlag, 2009, pp 591–614. [arXiv:0712.3318](http://arxiv.org/abs/0712.3318).
10. B. Nachtergaele, H. Raz, B. Schlein, and R. Sims, Commun. Math. Phys. 286, 1073–1098 (2009).
11. B. Nachtergaele, B. Schlein, R. Sims, S. Starr, and V. Zagrebnov, *On the existence of the dynamics for anharmonic quantum oscillator systems*, [arXiv:0909.2249](http://arxiv.org/abs/0909.2249).