Dispersion in infinite quantum systems

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Dispersion

- **Dispersion**: waves of different wavelengths have different propagation velocities

- **One quantum particle in vacuum**:

  \[ u(t, x) = e^{it\Delta}u_0 \] solves \[ i\partial_t u = -\Delta u \] with \[ u(0, x) = u_0(x) \]

  and spreads out like a melting snowman

- **Example**: coherent states

  \[ u_0 = \left(\pi\sigma^2\right)^{-d/4}e^{ip\cdot x}e^{-\frac{|x|^2}{2\sigma^2}} \] implies

  \[ |e^{it\Delta}u_0|^2 = \left(\pi\sigma(t)^2\right)^{-d/2}e^{-\frac{|x-2tp|^2}{\sigma(t)^2}} \]

\[ \sigma(t) := \sqrt{\sigma^2 + 4\frac{t^2}{\sigma^2}} \]
Dispersion in infinite quantum systems

- **New question:** starting with an infinite quantum systems close to equilibrium, will dispersion help to converge back to it for large times?

- **Application:** large-time stability of crystals close to equilibrium

- **Our work:**
  - infinitely extended Fermi gas
  - homogeneous (translation-invariant)
  - short range interactions
  - Kohn-Sham / Hartree-Fock theory, no exchange

**Difficulties:**
- infinitely many particles
- interacting with each other
Model

State of the system

**one-particle density matrix** = self-adjoint operator $0 \leq \gamma (\leq 1)$ acting on $L^2 (\mathbb{R}^d)$

Evolution of states: von Neumann equation

$$\begin{cases} 
i \partial_t \gamma &= \left[ -\Delta + w \ast \rho_{\gamma}, \gamma \right] \\ \gamma(0) &= \gamma_0 \end{cases}$$

- $w \in L^1 (\mathbb{R}) = \text{short range interaction}$
- $\rho_{\gamma} (x) = \gamma (x, x) = \text{density of particles in the system}$
- $w \ast \rho_{\gamma} = \int_{\mathbb{R}^d} w(x - y) \rho_{\gamma} (y) \, dy = \text{mean-field potential}$
- $N = \int_{\mathbb{R}^d} \rho_{\gamma} = \text{tr}(\gamma) = \text{total nb of particles}$
- $\gamma(t)$ unitarily equivalent to $\gamma_0$

**Example:** if $\gamma_0 = \sum_{j=1}^N \ket{u_{0,j}} \bra{u_{0,j}}$ then $\gamma(t) = \sum_{j=1}^N \ket{u_j(t)} \bra{u_j(t)}$ with

$$i \partial_t u_j = \left( -\Delta + w \ast \left( \sum_{k=1}^N |u_k|^2 \right) \right) u_j, \quad j = 1, \ldots, N$$
Homogeneous gas

Homogeneous gas with momentum distribution $g$

Translation-invariant $\gamma$

$\iff$ Fourier multiplier by $k \mapsto g(k) \in [0, 1]$

$\iff$ convolution kernel $\gamma(x, y) = (2\pi)^{-d/2} \hat{g}(x - y)$

Notation: $\gamma = g(-i\nabla)$

- constant density $\rho_{g(-i\nabla)} = (2\pi)^{-d/2} \hat{g}(0) = (2\pi)^{-d} \int_{\mathbb{R}^d} g(k) \, dk$
- $w \ast \rho_{g(-i\nabla)} = (2\pi)^{-d} \int_{\mathbb{R}^d} g \int_{\mathbb{R}^d} w \implies [-\Delta + w \ast \rho_{g(-i\nabla)}, g(-i\nabla)] \equiv 0$

If $w \in L^1(\mathbb{R}^d)$, any $\gamma = g(-i\nabla)$ with $g \in L^1(\mathbb{R}^d)$ is a stationary state!

Important physical examples:

$$g(k) = \mathbb{1}(|k|^2 \leq \mu)$$

| $g(k)$ | $\frac{1}{|k|^2 - \mu + 1}$ | $\frac{1}{|k|^2 - \mu - 1}$ | $e^{-\frac{|k|^2 - \mu}{T}}$
|---|---|---|---|
| Fermi gas | $T = 0$ | $\mu > 0$ | $T > 0$ | $\mu \in \mathbb{R}$
| Fermi gas | $T > 0$ | $\mu < 0$ | $T > 0$ | $\mu \in \mathbb{R}$
| Bose gas | $T > 0$ | $\mu \in \mathbb{R}$ | $T > 0$ | $\mu < 0$ | $T > 0$ | $\mu \in \mathbb{R}$

Mathieu LEWIN (CNRS / Cergy) Dispersion in infinite quantum systems Chicago, March 2014 5 / 13
Summary of results

\[
\begin{cases}
    i \partial_t \gamma &= \left[ -\Delta + w * \rho \gamma, \gamma \right] \\
    \gamma(0) &= g(-i\nabla) + Q_0
\end{cases}
\]

\[Q_0 = (\text{small?}) \text{ local perturbation}\]

- [LewSab-14a]: local + global existence, use relative (free) energy, \( T \geq 0 \)
- [LewSab-14a']: entropy bounds
- [LewSab-14b]: dispersion and scattering in 2D, \( T > 0 \)
- [FraLewLieSei-14]: new Strichartz inequality for operators


Equation for the perturbation

Let \( g \in L^1(\mathbb{R}^d, [0, 1]) \).

\( Q(t) := \gamma(t) - g(-i\nabla), \) the perturbation at time \( t \), solves

\[
\begin{cases}
  i \partial_t Q = \left[ -\Delta, Q \right] + \left[ w * \rho_Q, g(-i\nabla) \right] + \left[ w * \rho_Q, Q \right] \\
  Q(0) = Q_0
\end{cases}
\]

- \( Q(t) \) is not unitarily equivalent to \( Q_0 \)
- Even if \( Q_0 \) is finite-rank, \( Q(t) \) is never finite-rank for \( t > 0 \) because of the red term
- Competition between the 2 linear terms

Main difficulties:
- Which space for \( Q(t) \)? \( \rightsquigarrow \) Schatten spaces
- Proper definition of \( \rho_{Q(t)} \)? \( \rightsquigarrow \) new Strichartz
Schatten spaces

$Q$ self-adjoint compact operator with eigenvalues $\lambda_j$ and eigenvectors $(u_j)$:

$$
Q = \sum_j \lambda_j |u_j\rangle \langle u_j| \quad \iff \quad Q(x, y) = \sum_j \lambda_j u_j(x) \overline{u_j(y)}
$$

The $q$th Schatten norm is

$$
\|Q\|_{\mathcal{S}_q}^q := \sum_j |\lambda_j|^q = \text{tr}(|Q|^q), \quad |Q| = (Q^* Q)^{1/2}
$$

This spaces are included into one another

- **Density?**
  - $\rho_Q = \sum_j \lambda_j |u_j|^2$ is well defined in $L^1$ when $Q \in \mathcal{S}^1$
  - no clear definition of $\rho_Q$ if $Q \in \mathcal{S}^q$ with $q > 1$

**[LewSab-14a]:** local well-posedness in $\mathcal{S}^1$, but no scattering result
Strichartz inequality for orthonormal functions

**Theorem ([FraLewLieSei-14])**

Assume that $p, q, d \geq 1$ satisfy $1 \leq q \leq 1 + \frac{2}{d}$ and $\frac{2}{p} + \frac{d}{q} = d$. Then

$$\| \rho e^{it\Delta} Q e^{-it\Delta} \|_{L^p_t(L^q_x)} \leq C_{d,q} \| Q \|_{S^2 q/(q+1)}.$$ 

Equivalently, for any orthonormal system $(u_j)$ in $L^2(\mathbb{R}^d)$ and any $(\lambda_j) \subset \mathbb{C}$,

$$\left\| \sum_j \lambda_j |e^{it\Delta} u_j|^2 \right\|_{L^p_t(L^q_x)} \leq C_{d,q} \left( \sum_j |\lambda_j|^{\frac{2q}{q+1}} \right)^{\frac{q+1}{2q}}.$$ 

- usual Strichartz for one fn $\iff S^1$
- $(q + 1)/(2q)$ optimal for given $q$, cannot be increased (*semi-classics*)

[q 1 + \frac{2}{d} 1 + \frac{2}{d-1} 1 + \frac{2}{d-2}]

[FraLewLieSei-14] [FraSab-14] wrong!

usual Strichartz
Dispersion and scattering in 2D

**Theorem ([LewSab-14b])**

Assume that \( g \in W^{4,1}(\mathbb{R}^2, [0, 1]) \) is radial. Let \( w \in W^{1,1}(\mathbb{R}^2) \) be such that

\[
\| \hat{g} \|_{L^1(\mathbb{R}^2)} \| \hat{w} \|_{L^\infty(\mathbb{R}^2)} < 4\pi.
\]  

(1)

Then for \( \| Q_0 \|_{\mathbb{S}^{4/3}} \) small enough, the equation has a unique global solution, with

\[
\rho Q(t) = \rho \gamma(t) - \rho g(-i\nabla) \in L^2_{t,x}(\mathbb{R} \times \mathbb{R}^2)
\]

Moreover, \( \gamma(t) \) scatters around \( g(-i\nabla) \), in the sense that

\[
\lim_{t \to \pm \infty} \| e^{-it\Delta} \left( \gamma(t) - g(-i\nabla) \right) e^{it\Delta} - Q_\pm \|_{\mathbb{S}^4}
= \lim_{t \to \pm \infty} \| \gamma(t) - g(-i\nabla) - e^{it\Delta} Q_\pm e^{-it\Delta} \|_{\mathbb{S}^4} = 0
\]

for some \( Q_\pm \in \mathbb{S}^4 \).

**Rmk.** \( T > 0 \) covered, but not \( T = 0 \)
Strategy of proof: equation for $\rho_Q \in L^2_{t,x}$

- Duhamel’s formula

$$Q(t) = e^{it\Delta} Q_0 e^{-it\Delta} - i \int_0^t e^{i(t-t_1)\Delta} [w \ast \rho_Q(t_1), g(-i\nabla)] e^{i(t_1-t)\Delta} dt_1$$

Reinsert *ad infinitum* $\implies$ Dyson series in $\rho_Q$, with parameter $Q_0$

\[ \rho_Q(t) = \rho \left[ e^{it\Delta} Q_0 e^{-it\Delta} \right] - (\mathcal{L}_1[\rho] + \mathcal{L}_2[\rho_Q]) + \text{higher orders} \]

\[ \mathcal{L}_1[\rho] = \rho \left\{ i \int_0^t e^{i(t-t_1)\Delta} [w \ast \rho_Q(t_1), g(-i\nabla)] e^{i(t_1-t)\Delta} dt_1 \right\} \]

\[ \mathcal{L}_2[\rho] = \rho \left\{ i \int_0^t e^{i(t-t_1)\Delta} [w \ast \rho_Q(t_1), e^{it_1\Delta} Q_0 e^{-it_1\Delta}] e^{i(t_1-t)\Delta} dt_1 \right\} \]

\[ \rho_Q(t) = (1 + \mathcal{L})^{-1} \rho \left[ e^{it\Delta} Q_0 e^{-it\Delta} \right] + (1 + \mathcal{L})^{-1} \text{higher orders} \]

- $1 + \mathcal{L}$ invertible on $L^2_{t,x}$ $\oplus$ control higher orders $\implies$ $\rho_Q \in L^2_{t,x}$ (Banach fixed point)
- orders $\geq d + 1$ controlled similarly as for proof of Strichartz
The Linhard function

\[ \mathcal{L}_1[\rho] = \rho \left\{ i \int_0^t e^{i(t-t_1)\Delta} [w * \rho Q(t_1), g(-i \nabla)] e^{i(t_1-t)\Delta} dt_1 \right\} \]

is a space-time multiplier by

**Linhard function**

\[ m_g(\omega, k) = 2\hat{w}(k) \int_{\mathbb{R}} e^{-it\omega} \sin(t|k|^2) \tilde{g}(2tk) \, dt \]

**1 + \mathcal{L}_1 invertible \iff \min_{\omega,k} |1 + m_g(\omega, k)| > 0**

\[ |m_g(\omega, k)| \leq 2 \|\hat{w}\|_{L^\infty} \int_{\mathbb{R}} t|k|^2 \tilde{g}(2tk) \, dt \]

\[ = (4\pi)^{-1} \|\hat{w}\|_{L^\infty} \|\tilde{g}\|_{L^1} \]

\(\Re m_g\) always takes \(\leq 0\) and \(\geq 0\) values.

\(\Im m_g\) vanishes when \(\omega = 0\).

Plot of \(\Re m_g/\hat{w}\) for \(d = 2\), \(T = 100\) and \(\mu = 1\), in a neighborhood of \((\omega, |k|) = (0, 0)\)
Conclusion

- Return to equilibrium for an interacting homogeneous Fermi gas
- Strichartz inequality in Schatten spaces
- Linear response (Penrose type condition)

Many open problems!
- other dimensions
- $T = 0$?
- NLS ($w = c\delta$)
- convergence rates