Dispersion in infinite quantum systems

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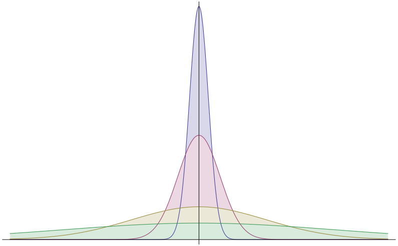
Dispersion

- **Dispersion:** waves of different wavelengths have different propagation velocities
- **One quantum particle in vacuum:**

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

and spreads out like a melting snowman

- **Example:** coherent states



Dispersion for one quantum particle in vacuum

$$u_0 = (\pi\sigma^2)^{-d/4} e^{ip\cdot x} e^{-\frac{|x|^2}{2\sigma^2}}$$

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

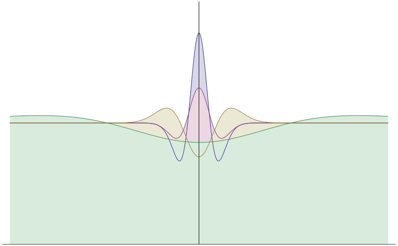
$$\sigma(t) := \sqrt{\sigma^2 + 4\frac{t^2}{\sigma^2}}$$

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:**



Return to equilibrium for an
infinitely extended homogeneous Fermi gas

- 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

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

- $w \in L^1(\mathbb{R})$ = short range interaction
- $\rho_\gamma(x) = \gamma(x,x)$ = density of particles in the system
- $w * \rho_\gamma = \int_{\mathbb{R}^d} w(x-y)\rho_\gamma(y)\,dy$ = mean-field potential
- $N = \int_{\mathbb{R}^d} \rho_\gamma = \mathrm{tr}(\gamma)$ = total nb of particles
- $\gamma(t)$ unitarily equivalent to γ_0

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

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

Homogeneous gas

Homogeneous gas with momentum distribution g

Translation-invariant γ

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

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

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

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

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) = $			
$\mathbb{1}(\lvert k\rvert^2 \leq \mu)$	$\dfrac{1}{e^{\frac{\lvert k\rvert^2-\mu}{T}}+1}$	$\dfrac{1}{e^{\frac{\lvert k\rvert^2-\mu}{T}}-1}$	$e^{-\frac{\lvert k\rvert^2-\mu}{T}}$
Fermi gas $T=0$ $\mu>0$	Fermi gas $T>0$ $\mu\in\mathbb{R}$	Bose gas $T>0$ $\mu<0$	Boltzmann $T>0$ $\mu\in\mathbb{R}$

Summary of results

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

$Q_0 =$ (small?) 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

[LewSab-14a] M.L. & J. Sabin. The Hartree equation for infinitely many particles. I. Well-posedness theory, *Comm. Math. Phys.*, 2014.

[LewSab-14b] M.L. & J. Sabin. The Hartree equation for infinitely many particles. II. Dispersion and scattering in 2D, *preprint arXiv*, 2013.

[LewSab-14a'] M.L. & J. Sabin. A family of monotone quantum relative entropies, *Lett. Math. Phys*, 2014.

[FraLewLieSei-14] R.L. Frank, M.L., E.H. Lieb & R. Seiringer. Strichartz inequality for orthonormal functions, *J. Eur. Math. Soc.*, 2014.

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

$$\begin{cases} i\,\partial_t Q = \underbrace{[-\Delta\,,\,Q] + [w*\rho_Q\,,\,g(-i\nabla)]}_{\text{linear}} + \underbrace{[w*\rho_Q\,,\,Q]}_{\text{nonlinear}} \\ Q(0) = Q_0 \end{cases}$$

- $Q(t)$ 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 λ_j and eigenvectors (u_j):

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

The qth Schatten norm is

$$\|Q\|_{\mathfrak{S}^q}^q := \sum_j |\lambda_j|^q = \operatorname{tr}(|Q|^q), \qquad |Q| = (Q^*Q)^{1/2}$$

This spaces are included into one another

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

[LewSab-14a]: local well-posedness in $\mathfrak{S}^1$, but no scattering result

Strichartz inequality for orthonormal functions

Theorem ([FraLewLieSei-14])

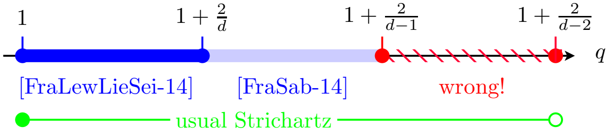
Assume that $p, q, d \geq 1$ *satisfy* $1 \leq q \leq 1 + \frac{2}{d}$ *and* $\frac{2}{p} + \frac{d}{q} = d$. *Then*

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

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

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

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



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*

$$\|\check{g}\|_{L^1(\mathbb{R}^2)} \|\widehat{w}\|_{L^\infty(\mathbb{R}^2)} < 4\pi. \tag{1}$$

Then for $\|Q_0\|_{\mathfrak{S}^{4/3}}$ *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*

$$\lim_{t\to\pm\infty} \left\| e^{-it\Delta}\big(\gamma(t) - g(-i\nabla)\big)e^{it\Delta} - Q_\pm \right\|_{\mathfrak{S}^4} = \lim_{t\to\pm\infty} \Big\| \gamma(t) - g(-i\nabla) - \underbrace{e^{it\Delta} Q_\pm e^{-it\Delta}}_{\rightharpoonup 0} \Big\|_{\mathfrak{S}^4} = 0$$

for some $Q_\pm \in \mathfrak{S}^4$.

Rmk. $T > 0$ covered, but not $T = 0$

Strategy of proof: equation for $\rho_Q \in L^2_{t,x}$

- **Duhamel's formula**

$$Q(t) = e^{it\Delta}Q_0e^{-it\Delta} - i\int_0^t e^{i(t-t_1)\Delta}[w*\rho_Q(t_1), g(-i\nabla) + \underbrace{Q(t_1)}_{?}]e^{i(t_1-t)\Delta}dt_1$$

Reinsert *ad infinitum* $\Longrightarrow$ Dyson series in ρ_Q, with parameter Q_0

$$\rho_Q(t) = \underbrace{\rho[e^{it\Delta}Q_0e^{-it\Delta}]}_{\text{Strichartz}} - \underbrace{(\mathcal{L}_1[\rho] + \mathcal{L}_2[\rho_Q])}_{\mathcal{L}[\rho_Q]} + \text{higher orders}$$

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

$$\mathcal{L}_2[\rho] = \rho\left\{i\int_0^t e^{i(t-t_1)\Delta}[w*\rho_Q(t_1), e^{it_1\Delta}Q_0e^{-it_1\Delta}]e^{i(t_1-t)\Delta}dt_1\right\}$$

$$\rho_Q(t) = (1+\mathcal{L})^{-1}\rho[e^{it\Delta}Q_0e^{-it\Delta}] + (1+\mathcal{L})^{-1}\text{higher orders}$$

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

The Linhard function

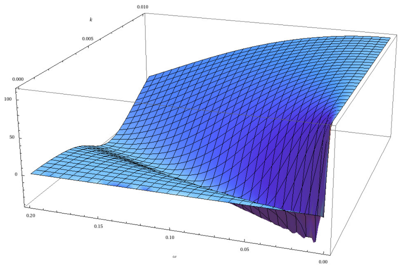
$$\mathcal{L}_1[\rho] = \rho\left\{ i\int_0^t e^{i(t-t_1)\Delta}[w*\rho_Q(t_1), g(-i\nabla)]e^{i(t_1-t)\Delta}dt_1\right\}$$

is a space-time multiplier by

Linhard function

$$m_g(\omega,k) = 2\widehat{w}(k)\int_{\mathbb{R}} e^{-it\omega}\sin(t|k|^2)\check{g}(2tk)\,dt$$

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



$$|m_g(\omega,k)| \leq 2\,\|\widehat{w}\|_{L^\infty}\int_{\mathbb{R}} t|k|^2\check{g}(2tk)\,dt = (4\pi)^{-1}\,\|\widehat{w}\|_{L^\infty}\,\|\check{g}\|_{L^1}$$

$\Re\, m_g$ always takes ≤ 0 and ≥ 0 values

$\Im\, m_g$ vanishes when $\omega = 0$

Plot of $\Re\, m_g/\widehat{w}$ 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