The Mean-Field Limit for the Quantum N-Body Problem: Uniform in $\hbar$ Convergence Rate

François Golse

CMLS, École polytechnique & CNRS, Université Paris-Saclay

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Work with T. Paul and M. Pulvirenti

Motivation

•The Hartree equation with bounded interaction potential has been derived from the N-body linear Schrödinger equation in the large N, small coupling constant limit (Spohn 80, Bardos-FG-Mauser 2000, Rodnianski-Schlein 09); extension to singular interaction potentials (including Coulomb) by Erdös-Yau 2001, Pickl 2009. The convergence rate obtained in these works is not uniform as $\hbar \to 0 \ldots$

•…and yet the Vlasov equation with $C^{1,1}$ interaction potential has been derived from the N-body problem of classical mechanics in the same limit (Neunzert-Wick 1973, Braun-Hepp 1977, Dobrushin 1979)

Problem: to find a uniform in $\hbar$ convergence rate for the quantum mean-field limit (Graffi-Martinez-Pulvirenti M3AS03, Pezzotti-Pulvirenti AnnHP09, G-Mouhot-Paul CMP2016)

The diagram

Schrödinger	$\stackrel{N\to\infty}{\longrightarrow}$	**Hartree**
$\downarrow$		$\downarrow$
$\hbar \to 0$		$\hbar \to 0$
$\downarrow$		$\downarrow$
Liouville	$\stackrel{N\to\infty}{\longrightarrow}$	**Vlasov**

THE QUANTUM N-BODY PROBLEM

Hartree equation

= a nonlinear, nonlocal Schrödinger equation on the 1-particle space $\mathfrak{H} = L^2(\mathbf{R}^d)$ for the "typical" particle interacting with a large number of other identical particles

Mean-field interaction potential and Hamiltonian:

$$V_{\rho(t)}(x) := \int_{\mathbf{R}^d} V(x-y)\rho(t,y,y)dy\,, \quad \mathbf{H}_{\rho(t)} := -\tfrac{1}{2}\hbar^2\Delta + V_{\rho(t)}$$

•The 1-body wave function $\psi \equiv \psi(t,x)$ satisfies Hartree's equation

$$i\hbar\partial_t\psi = \mathbf{H}_{|\psi\rangle\langle\psi|(t)}\psi\,, \quad \psi\big|_{t=0} = \psi^{in}$$

Density formulation the 1-body density operator $\rho \equiv \rho(t)$ satisfies

$$i\hbar\partial_t\rho(t) = [\mathbf{H}_{\rho(t)}, \rho(t)]\,, \quad \rho\big|_{t=0} = \rho^{in}$$

N-Body Schrödinger

Notation for a N-tuple of positions is $X_N := (x_1, \ldots, x_N) \in (\mathbf{R}^d)^N$

•The N-body wave function $\Psi_N \equiv \Psi_N(t, x_1, \ldots, x_N) \in \mathbf{C}$ satisfies the N-**body Schrödinger equation**

$$i\hbar\partial_t\Psi_N = \mathcal{H}_N\Psi_N\,, \quad \mathcal{H}_N := \sum_{j=1}^{N} -\tfrac{1}{2}\hbar^2\Delta_{x_j} + \frac{1}{N}\sum_{1\le j<k\le N} V(x_j - x_k)$$

Action of the symmetric group: for each permutation $\sigma \in \mathfrak{S}_N$

$$U_\sigma\Psi_N(X_N) := \Psi_N(\sigma\cdot X_N) \quad \text{where } \sigma\cdot X_N := (x_{\sigma^{-1}(1)}, \ldots, x_{\sigma^{-1}(N)})$$

N-Body Heisenberg

• The N-body density operator $\rho_N(t) := |\Psi_N(t,\cdot)\rangle\langle\Psi_N(t,\cdot)|$ satisfies the N-**body Heisenberg equation**

$$i\hbar\partial_t\rho_N = [\mathcal{H}_N, \rho_N], \quad \rho_N\big|_{t=0} = \rho_N^{in}$$

Density operators: set $\mathfrak{H} := L^2(\mathbf{R}^d)$ and $\mathfrak{H}_N = \mathfrak{H}^{\otimes N} \simeq L^2((\mathbf{R}^d)^N)$

$$\mathcal{D}(\mathfrak{H}_N) := \{\rho \in \mathcal{L}(\mathfrak{H}_N) \text{ s.t. } \rho = \rho^* \geq 0 \text{ and } \operatorname{tr}(\rho) = 1\}$$

Indistinguishable particles $\Leftrightarrow$ symmetric density operators

$$\mathcal{D}^s(\mathfrak{H}_N) := \{\rho \in \mathcal{D}(\mathfrak{H}_N) \text{ s.t. } \rho = U_\sigma\rho U_\sigma^* \quad \text{for each } \sigma \in \mathfrak{S}_N\}$$

• **Propagation of symmetry** by the N-body Heisenberg equation:

$$\rho_N^{in} \in \mathcal{D}^s(\mathfrak{H}_N) \Rightarrow \rho_N(t) \in \mathcal{D}^s(\mathfrak{H}_N) \text{ for all } t \geq 0$$

THE BBGKY HIERARCHY FORMALISM

Marginals

***k*-particle marginal of a density operator:** for $\rho_N \in \mathcal{D}^s(\mathfrak{H}_N)$, and for $1 \leq k \leq N$, define $\rho_N^{\mathbf{k}} \in \mathcal{D}^s(\mathfrak{H}_k)$ by the identity

$$\mathrm{tr}_{\mathfrak{H}_k}(\rho_N^{\mathbf{k}} A) = \mathrm{tr}_{\mathfrak{H}_N}(\rho_N(A \otimes I_{\mathfrak{H}_{N-k}})) \qquad \text{for each } A \in \mathcal{L}(\mathfrak{H}_k)$$

•The integral kernel of $\rho_N^{\mathbf{k}}$ is defined in terms of the integral kernel of ρ_N by the formula

$$\rho_N^{\mathbf{k}}(X_k, Y_k) = \int_{(\mathbf{R}^d)^{N-k}} \rho_N(X_k, Z_{N-k}, Y_k, Z_{N-k}) dZ_{N-k}$$

BBGKY hierarchy

Pbm: to find an equation for $\rho_N^{\mathbf{k}}$ knowing that ρ_N is a solution to the Heisenberg equation, where $k = 1, \ldots, N$

$$i\hbar\partial_t \rho_N^{\mathbf{k}} = [-\tfrac{1}{2}\hbar^2\Delta^{\mathbf{k}}, \rho_N^{\mathbf{k}}]$$

$$+ \underbrace{\frac{N-k}{N}\sum_{j=1}^{k}\left[V_{j,k+1}, \rho_N^{\mathbf{k+1}}\right]^{\mathbf{k}}}_{\text{interaction with the } N-k \text{ other particles}} + \underbrace{\frac{1}{N}\sum_{1\le m<n\le k}[V_{m,n}, \rho_N^{\mathbf{k}}]}_{\text{recollision}}$$

Notation:

$$V_{m,n} := \text{ multiplication by } V(x_m - x_n)\,, \qquad \Delta^{\mathbf{k}} := \sum_{j=1}^{k}\Delta_{x_j}$$

The Hartree hierarchy

If $\rho \equiv \rho(t)$ is a solution to the Hartree equation, the sequence $\rho_k(t) := \rho(t)^{\otimes k}$ satisfies the infinite hierarchy of equations

$$i\hbar\partial_t\rho_k = [-\tfrac{1}{2}\hbar^2\Delta^{\mathbf{k}}, \rho_k] + \sum_{j=1}^{k} \underbrace{[V_{j,k+1}, \rho_{k+1}]^{\mathbf{k}}}_{=[V_{\rho(t)}(x_j),\rho_k(t)]}$$

Setting $E_{N,k}(t) := \rho_k(t) - \rho_N^{\mathbf{k}}(t)$, one finds that

$$i\hbar\partial_t E_{N,k} = [-\tfrac{1}{2}\hbar^2\Delta^{\mathbf{k}}, E_{N,k}] + \sum_{j=1}^{k}[V_{j,k+1}, E_{N,k+1}]^{\mathbf{k}}$$

$$+ \underbrace{\frac{k}{N}\sum_{j=1}^{k}\left[V_{j,k+1}, \rho_N^{\mathbf{k}}\right]^{\mathbf{k}}}_{O(k^2/N)} - \underbrace{\frac{1}{N}\sum_{1\le m<n\le k}[V_{m,n}, \rho_N^{\mathbf{k}}]}_{O(k^2/N)}$$

A nonuniform convergence rate in trace norm

Thm I Assume that $V \in L^\infty(\mathbf{R}^d)$ is even and real-valued. Assume that the initial data for the N-body Heisenberg equation is factorized

$$\rho_N\Big|_{t=0} = (\rho^{in})^{\otimes N}$$

where ρ^{in} is the initial data for the Hartree equation. Then

$$\mathrm{tr}(|\rho_N^{\mathbf{k}}(t) - \rho(t)^{\otimes k}|) \leq 2^k \frac{2^{1+16Wt/\hbar}}{N^{\ln 2/2^{1+16Wt/\hbar}}}$$

for all $t \geq 0$, all $k \geq 1$ and all $N \geq \max\left(N_0(k), \exp\left(2^{1+16Wt/\hbar}k\right)\right)$, where

$$N_0(k) := \inf\{N > e^4 \text{ s.t. } n \geq N \Rightarrow 2^{\ln n/2}(k + \tfrac{1}{2}\ln n)^2 < 2n\}$$

and

$$W := \|V\|_{L^\infty(\mathbf{R}^d)}$$

THE OPTIMAL TRANSPORT FORMALISM

Monge-Kantorovich-(Vasershtein-Rubinshtein) distances

Let μ, ν be two Borel probability measures on $\mathbf{R}^d$.

Coupling of μ, ν: a Borel measure $\pi \geq 0$ on $\mathbf{R}^d \times \mathbf{R}^d$ such that

$$\iint_{\mathbf{R}^d \times \mathbf{R}^d} (\phi(x)+\psi(y))\pi(dxdy) = \int_{\mathbf{R}^d} \phi(x)\mu(dx) + \int_{\mathbf{R}^d} \psi(y)\nu(dy)$$

for all $\phi, \psi \in C_b(\mathbf{R}^d)$.

Set of couplings of μ, ν denoted $\Pi(\mu, \nu)$

Monge-Kantorovich distance (exponent $p \geq 1$):

$$\mathrm{dist}_{MK,p}(\mu,\nu) = \left(\inf_{\pi \in \Pi(\mu,\nu)} \iint_{\mathbf{R}^d \times \mathbf{R}^d} |x-y|^p \pi(dxdy) \right)^{1/p}$$

Quantum couplings and pseudo-distance

•Density operators on a Hilbert space $\mathfrak{H}$:

$$\rho \in \mathcal{D}(\mathfrak{H}) \Leftrightarrow \rho = \rho^* \geq 0\,, \quad \operatorname{tr}(\rho) = 1$$

•Couplings between two density operators $\rho_1, \rho_2 \in \mathcal{D}(\mathfrak{H})$:

$$\rho \in \mathcal{D}(\mathfrak{H} \otimes \mathfrak{H}) \text{ s.t. } \left\{ \begin{array}{l} \operatorname{tr}_{\mathfrak{H}\otimes\mathfrak{H}}((A \otimes I)\rho) = \operatorname{tr}_{\mathfrak{H}}(A\rho_1) \\ \operatorname{tr}_{\mathfrak{H}\otimes\mathfrak{H}}((I \otimes A)\rho) = \operatorname{tr}_{\mathfrak{H}}(A\rho_2) \end{array} \right.$$

for all $A \in \mathcal{L}(\mathfrak{H})$; the set of all such ρ will be denoted $\mathcal{Q}(\rho_1, \rho_2)$
•For $\rho_1, \rho_2 \in \mathcal{D}(L^2(\mathbf{R}^d))$, define

$$MK_2^\hbar(\rho_1, \rho_2) = \inf_{\rho \in \mathcal{Q}(\rho_1, \rho_2)} \operatorname{tr}\left(\sum_{j=1}^d ((x_j - y_j)^2 - \hbar^2(\partial_{x_j} - \partial_{y_j})^2)\rho \right)^{1/2}$$

Thm II [FG - C. Mouhot - T. Paul, CMP2016]
Let the potential V be even, real-valued and s.t. $\nabla V \in \mathrm{Lip}(\mathbf{R}^d)$.

Let $\rho_\hbar(t)$ be the solution of Hartree's equation with initial data $\rho_\hbar^{in}$, and let $\rho_{N,\hbar}(t)$ be the solution of Heisenberg's equation with initial data $\rho_{N,\hbar}^{in} \in \mathcal{D}^s(\mathfrak{H}_N)$.

Then, for each $t \geq 0$

$$MK_2^\hbar(\rho_\hbar(t), \rho_{N,\hbar}^{\mathbf{1}}(t))^2 \leq \frac{1}{N} MK_2^\hbar((\rho_\hbar^{in})^{\otimes N}, \rho_{N,\hbar}^{in})^2 e^{Lt} + \frac{8}{N}\|\nabla V\|_{L^\infty}^2 \frac{e^{Lt}-1}{L}$$

with

$$L := 3 + 4\,\mathrm{Lip}(\nabla V)^2$$

Dynamics of quantum couplings

Let $R_N^{in} \in \mathcal{Q}((\rho^{in})^{\otimes N}, \rho_N^{in})$ and let $t \mapsto R_N(t)$ be the solution of

$$i\hbar\partial_t R_N = \left[\sum_{k=1}^{N} \mathbf{H}^k_{\rho(t)} \otimes I + I \otimes \mathcal{H}_N, R_N\right], \quad R_N\big|_{t=0} = R_N^{in}$$

Then $R_N(t) \in \mathcal{Q}((\rho(t))^{\otimes N}, \rho_N(t))$ for each $t \geq 0$. Define

$$D_N(t) = \operatorname{tr}\left(\frac{1}{N}\sum_{j=1}^{N}(Q_j^* Q_j + P_j^* P_j) R_N(t)\right)$$

with

$$Q_j = x_j - y_j\,, \quad P_j := \tfrac{\hbar}{i}(\nabla_{x_j} - \nabla_{y_j})\,, \quad P_j^* := \tfrac{\hbar}{i}(\operatorname{div}_{x_j} - \operatorname{div}_{y_j})$$

Ideas from the proof

Need to control the operator

$$\left[\sum_{k=1}^{N} \mathbf{H}^{k}_{\rho(t)} \otimes I + I \otimes \mathcal{H}_N, Q_1^* Q_1 + P_1^* P_1\right]$$

in terms of

$$\frac{1}{N}\sum_{j=1}^{N}(Q_j^* Q_j + P_j^* P_j)$$

and

$$\operatorname{tr}\left(\left|V_{\rho(t)} - \frac{1}{N}\sum_{k=1}^{N} V(\cdot - x_k)\right|^2 \rho_\hbar(t)^{\otimes N}\right) = O(1/N)$$

Both steps use the Lipschitz continuity of ∇V

PROPERTIES OF $MK_2^\hbar$

Wigner and Husimi transforms

•**Wigner transform** at scale $\hbar$ of an operator $\rho \in \mathcal{D}(L^2(\mathbf{R}^d))$:

$$W_\hbar[\rho](x,\xi) = \frac{1}{(2\pi)^d} \int_{\mathbf{R}^d} e^{-i\xi\cdot y} \rho(x + \tfrac{1}{2}\hbar y, x - \tfrac{1}{2}\hbar y) dy$$

•**Husimi transform** at scale $\hbar$:

$$\tilde{W}_\hbar[\rho](x,\xi) = e^{\hbar\Delta_{x,\xi}/4} W_\hbar[\rho] \geq 0$$

One has

$$\int_{\mathbf{R}^d \times \mathbf{R}^d} \tilde{W}_\hbar[\rho](x,\xi) dx d\xi = \mathrm{tr}(\rho) = 1$$

Töplitz quantization

•**Coherent state** with $q, p \in \mathbf{R}^d$:

$$|q + ip, \hbar\rangle = (\pi\hbar)^{-d/4} e^{-|x-q|^2/2\hbar} e^{ip\cdot x/\hbar}$$

•With the identification $z = q + ip \in \mathbf{C}^d$

$$\mathrm{OP}^T(\mu) := \tfrac{1}{(2\pi\hbar)^d} \int_{\mathbf{C}^d} |z, \hbar\rangle\langle z, \hbar| \mu(dz)\,, \quad \mathrm{OP}^T(1) = I$$

•Fundamental properties:

$$\mu \geq 0 \Rightarrow \mathrm{OP}^T(\mu) \geq 0\,, \quad \mathrm{tr}(\mathrm{OP}^T(\mu)) = \tfrac{1}{(2\pi\hbar)^d} \int_{\mathbf{C}^d} \mu(dz)$$

•Important formulas:

$$W_\hbar[\mathrm{OP}^T(\mu)] = \tfrac{1}{(2\pi\hbar)^d} e^{\hbar\Delta_{q,p}/4}\mu\,, \quad \tilde{W}_\hbar[\mathrm{OP}^T(\mu)] = \tfrac{1}{(2\pi\hbar)^d} e^{\hbar\Delta_{q,p}/2}\mu$$

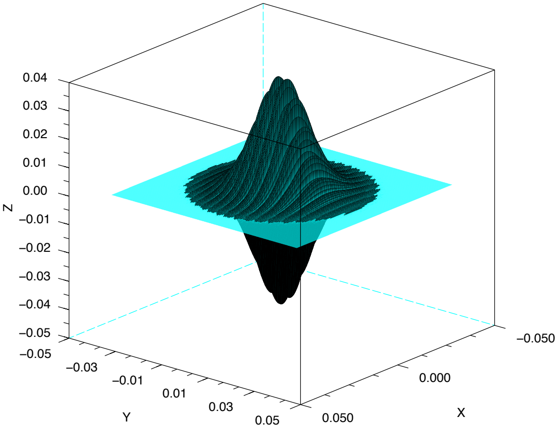

Figure: With $\hbar = 8 \cdot 10^{-5}$, Z =real part of coherent state centered at $q = (0, 0)$ with momentum $p = (1, 0)$ with space variable $(X, Y) \in \mathbf{R}^2$

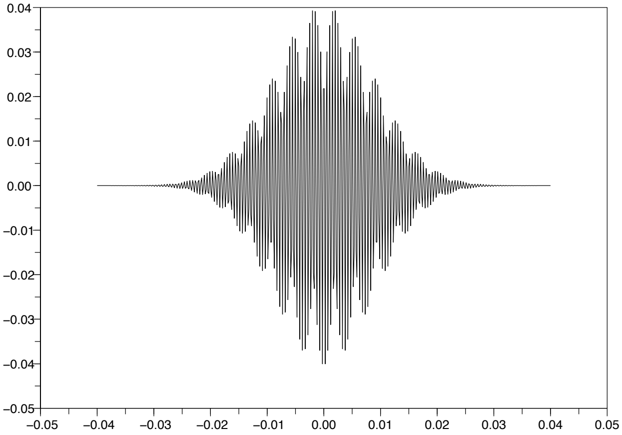

Figure: Oscillating structure of a Gaussian coherent state.

Comparing $MK_2^\hbar$ with $\mathrm{dist}_{\mathrm{MK},2}$

Thm III [FG - C. Mouhot - T. Paul, CMP2016]
(a) $MK_2^\hbar$ is **not a distance**: for all $\rho_1, \rho_2 \in \mathcal{D}(L^2(\mathbf{R}^d))$, one has

$$MK_2^\hbar(\rho_1,\rho_2)^2 \geq \max(2d\hbar, \mathrm{dist}_{\mathrm{MK},2}(\tilde{W}_\hbar[\rho_1], \tilde{W}_\hbar[\rho_2])^2 - 2d\hbar)$$

(b) Let ρ_j be the Töplitz operators at scale $\hbar$ with symbol $(2\pi\hbar)^d\mu_j$, with $\mu_j \in \mathcal{P}_2(\mathbf{C}^d)$ for $j = 1, 2$; then

$$MK_2^\hbar(\rho_1,\rho_2)^2 \leq \mathrm{dist}_{\mathrm{MK},2}(\mu_1,\mu_2)^2 + 2d\hbar$$

Notation: $\mathcal{P}(\mathbf{R}^d) =$ set of Borel probability measures on $\mathbf{R}^d$, and

$$\mathcal{P}_n(\mathbf{R}^d) := \left\{ \mu \in \mathcal{P}(\mathbf{R}^d) \text{ s.t. } \int_{\mathbf{R}^d} |x|^n \mu(dx) < \infty \right\}$$

Corollary

Let the potential V be even, real-valued and s.t. $\nabla V \in W^{1,\infty}(\mathbf{R}^d)$. Let $\rho_\hbar(t)$ be the solution of the Hartree equation with initial data ρ^{in}, assumed to be a Töplitz density operator. Let $\rho_{N,\hbar}(t)$ be the solution of the N-body Heisenberg equation with initial data $(\rho^{in})^{\otimes N}$. Then

$$\operatorname{dist}_{\mathrm{MK},2}(\tilde{W}_\hbar[\rho^{\mathbf{1}}_{N,\hbar}(t)], \tilde{W}_\hbar[\rho_\hbar(t)])^2$$
$$\leq 2d\hbar(e^{Lt}+1) + \frac{8}{N}\|\nabla V\|^2_{L^\infty}\frac{e^{Lt}-1}{L}$$

•Convergence rate as $N \to \infty$ that is uniform as $\hbar \to 0$...

•... but this estimate says nothing for $\hbar$ fixed

THE INTERPOLATION ARGUMENT

Lemma:

(1) Let $\rho_1, \rho_2 \in \mathcal{D}(\mathfrak{H})$; then

$$\left\| \widetilde{W_\hbar}[\rho_1] - \widetilde{W_\hbar}[\rho_2] \right\|_{TV} \leq \mathrm{tr}(|\rho_1 - \rho_2|)$$

(2) Let $\mu, \nu \in \mathcal{P}(\mathbf{R}^d)$ and $\Pi(\mu,\nu)$ be the set of couplings of μ, ν. Define

$$\mathrm{dist}_1(\mu,\nu) = \inf_{\pi \in \Pi(\mu,\nu)} \iint_{\mathbf{R}^d \times \mathbf{R}^d} \min(1, |x-y|)\pi(dxdy)$$

Then

$$\mathrm{dist}_1(\mu,\nu) \leq \min(\|\mu - \nu\|_{TV}, \mathrm{dist}_{\mathrm{MK},2}(\mu,\nu))$$

Thm IV

Let the potential $V \in C^{1,1}(\mathbf{R}^d)$ be even and real-valued.

Let $\rho_\hbar(t)$ be the solution of the Hartree equation with Töplitz initial data $\rho_\hbar^{in} \in \mathcal{D}(\mathfrak{H})$, and let $\rho_{N,\hbar}(t)$ be the solution of Heisenberg's equation with initial data $(\rho_\hbar^{in})^{\otimes N}$.

Then, for each $t^* \geq 0$, one has

$$\sup_{0 \leq t \leq t^*} \operatorname{dist}_1(\widetilde{W}_\hbar[\rho_\hbar(t)], \widetilde{W}_\hbar[\rho^{\mathbf{1}}_{N,\hbar}(t)])^2 \lesssim 64 dW \ln 2 \frac{t^*(1+e^{Lt^*})}{\ln \ln N}$$

where

$$W := \|V\|_{L^\infty(\mathbf{R}^d)} \qquad \text{and} \qquad L := 3 + 4\,\mathrm{Lip}(\nabla V)^2$$

Key idea

•Use the BBGKY estimate (Theorem I) for $\hbar > O(1/\ln\ln N)$

•Use the optimal transport estimate (Theorem II+III) otherwise

Conclusion

•Uniform in $\hbar$ convergence rate for the mean-field limit of the N-body quantum problem with factorized initial data

•Formulated in terms of the Dobrushin weak convergence distance on Husimi transforms of the Hartree solution and of the 1st marginal of the N-body density operator

•Decay of order $O(1/\sqrt{\ln \ln N})$ most likely non optimal, due to the finite time (Cauchy-Kowalevski) limitation in the stability of the BBGKY hierarchy

Other approaches avoiding BBGKY hierarchies?

•2nd quantization (Rodnianski-Schlein CMP2007, error of order e^{Kt}/N in trace norm, K not explicit...)

Open questions

•In classical mechanics, the N-particle phase space empirical measure is a weak solution of the mean-field (Vlasov) equation. Is there a quantum analogue of this property? (work in progress on that question with T. Paul...)

•Is there a Benamou-Brenier type variational formulation for the pseudo-distance $MK_2^\hbar$?

•Can one replace $MK_2^\hbar$ with a true distance? (for instance, Connes' distance in NC geometry, which is the analogue for operator algebras of the MK distance with exponent 1)

Two of Yann's interests: Switzerland and locomotives

Figure: A. Honegger and a Pacific 231 steam locomotive

"I have always loved locomotives passionately. For me they are living creatures and I love them as others love women or horses."

A. Honegger

Finally, the most important slide in this talk

HAPPY BIRTHDAY, YANN !