On a classical limit of quantum theory and the non-linear Hartree equation ‡

Jürg Fröhlich
Theoretical Physics, ETH-Hönggerberg, CH–8093 Zürich, Switzerland

Tai-Peng Tsai and Horng-Tzer Yau
Courant Institute of Mathematical Sciences, New York University
251 Mercer Street, New York, NY 10471, USA

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Dedicated to the memory of Moshé Flato, whose contributions to deformation quantization are fundamental

1. General perspective, description of the problem

Historically, the description of Nature in theoretical physics began with an encoding of rather special, simple natural phenomena exhibiting high approximate symmetry in special, unstable mathematical structures. For example, the shape of the orbits of planets around the sun was conceived to be circular. As the ambition to describe more general classes of natural phenomena grew those special mathematical structures had to be deformed and enlarged into more general, more stable mathematical structures. Kepler discovered that the idea of elliptic orbits, with the sun in one of the foci, provides a better model for the motion of planets.

With the advent of the idea of *dynamical* Laws of Nature, one discovered that it is these laws that may exhibit high symmetry, rather than special consequences of these laws. Newtonian mechanics led to a first model of space and time. The orbits of planets and moons could be understood as trajectories in Newtonian space-time which are solutions of the Newtonian equations of motion. These equations of motion exhibit high symmetry: In all inertial frames of reference they take the same form, the transition from one to another inertial frame being given by a Galilei transformation. These symmetries are accompanied by conservation laws.

During the twentieth century, our understanding of Nature underwent revolutionary developments and changes which led to at least three fundamental *deformations* of the mathematical structure underlying physical theory. The first one

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originated from the study of the laws of black-body radiation and resulted in the discovery of *quantum theory*. As early as 1900, it uncovered new fundamental constants of Nature, the elementary electric charge e, the Boltzmann constant k_B, Planck's constant $\hbar$ — all related to the atomic constitution of matter — and the Planck length ℓ_P which is connected with gravity. Planck's law of black-body radiation, combined with previously discovered laws of thermodynamics and statistical physics, enabled him to determine the approximate values of e, k_B and $\hbar$, and from the speed of light c, and Newton's law of gravitational attraction he could then infer the approximate value of ℓ_P.

The second revolution arose from attempts to find a unified description of mechanical and electromagnetic phenomena and resulted in Einstein's special theory of relativity and in the deformation of Newtonian space-time to Minkowski space-time and of the Galilei group to the Poincaré group. The underlying deformation parameter is the speed of light c. The third one arose from trying to find a relativistic theory of gravitation and an invariant (coordinate-independent) formulation of fundamental dynamical laws and resulted in Einstein's general theory of relativity. In this theory, Minkowski space-time is deformed to a dynamical space-time, described as a Lorentzian manifold, whose topology and metric shape are determined, in part, by the distribution of matter. *Global* space-time symmetries are promoted to *local* symmetries (gauge symmetries of the second kind). The underlying deformation parameter is ℓ_P.

The deformation of the mathematical structure underlying Hamiltonian mechanics to the one underlying non-relativistic quantum mechanics was accomplished last and has remained, perhaps, the most mysterious one. The underlying deformation parameter is Planck's constant $\hbar$. It represents the first example of a deformation of classical geometry to noncommutative geometry, namely the deformation of symplectic geometry to the noncommutative geometry of quantized phase spaces.

The three deformations mentioned above and their diverse fundamental physical consequences have set much of the agenda for the theoretical physics of the twentieth century and are likely to occupy an important place in our agenda for many years to come.

Moshé Flato was very actively involved in research on deformation theory and made or stimulated fundamental contributions in this area. His insights in this and many other developments will be missed!

From the experience gained from the deformations of Newtonian to relativistic mechanics, of special to general relativity and of Hamiltonian to quantum mechanics, one may infer that *dimensionful, fundamental constants of Nature*, c, $\hbar$, ℓ_P, play the role of *deformation parameters*, (to be distinguished from scale hierarchy parameters, such as the Rydberg, the QCD scale or the mass of the Z boson, and from dimensionless coupling constants, such as the fine structure constant $\alpha \simeq 1/137$, or Yukawa couplings). To "turn on" $1/c$ or $\hbar$ or ℓ_P necessitates a fundamental change in the mathematical structure of physical theory, the passage

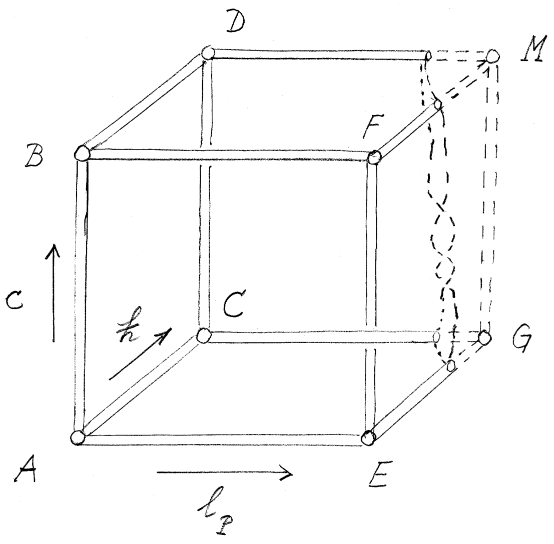

Figure 1.

from one family to a new family of theories, (while ratios of energy scales and dimensionless coupling constants can be viewed as *moduli* parametrizing a family of theories). Dimensionful, fundamental constants of nature permit us to introduce a natural system of units in which they take the value 1, i.e., $c = 1$, $\hbar = 1$ and $\ell_P = 1$, in natural units, (while ratios of energy scales and dimensionless coupling constants are pure numbers independent of our choice of units).

Deforming one family of theories to a new family of theories is the subject of *deformation theory*, while the passage from an effective description of natural phenomena at a high energy scale to an effective description of phenomena at a lower energy scale (within one family of effective theories) is the subject of *renormalization group theory*. Deformation theory is algebra, renormalization group theory is analysis. Progress in theoretical physics appears to rely on progress in deformation — and in renormalization group theory!

The sketch in Figure 1 may convey a very rough impression of where we stand, at present:

A. Newtonian mechanics, Euclidian geometry, Hamiltonian mechanics, symplectic geometry

B. Special relativistic classical field theory, Minkowski geometry, infinite-dimensional symplectic geometry

C. Non-relativistic quantum mechanics, noncommutative geometry of quantized phase spaces

D. Special relativistic quantum field theory, noncommutative geometry of infinite-dimensional quantized phase spaces, functional integration, BRST- and BV cohomology

E. Newtonian gravity and its reformulation as a geometrical theory, making use of Riemannian geometry

F. General Relativity, general Lorentzian geometry, ...

G. "Non-relativistic quantum gravity" (?), noncommutative Riemannian geometry

M. "Quantum gravity" or "M-theory" (?), infinite-dimensional noncommutative differential geometry (?), ...

The question marks indicate that the corresponding terms do not have a mathematically precise definition, yet. The "Escherian" aspect of the cube in Figure 1 is intended to indicate that we are still facing obstacles or, perhaps, obstructions in attempting to add the missing vertices G and M, and a link between them, to the cube.

Our discussion makes it clear that the following have been and will remain *important tasks* for theoretical physicists:

(1) Find suitable stable mathematical structures as foundations for physical theory by *deforming* more special, less stable mathematical structures known to underly physical theory in various asymptotic regimes.

For the future (ℓ_P): Find the deformations leading to vertex G and, most importantly, to vertex M, ("M-theory").

(2) Once a physical theory founded on a general, stable mathematical structure (e.g., non-relativistic quantum mechanics) has been found, one must understand in which asymptotic regime it reduces to one of its ancestor theories (e.g., Hamiltonian mechanics) founded on a less stable structure from which the former has arisen by deformation.

For the future (length scales $\gg \ell_P$):

$$\begin{tikzcd} \boxed{\text{“M-theory”}} \arrow[r, "\text{compact dimensions, D-branes,...}"'] & \boxed{\begin{array}{l}\text{special relativistic}\\ \text{quantum field theory}\end{array}} \end{tikzcd}$$

We do not really know precisely what "M-theory" is, and we do not understand how as yet unobserved symmetries (in particular, space-time supersymmetry) are broken and how a hierarchy of low-energy scales is generated.

For now ($c \gg$ typical velocities):

(i) special relativistic quantum field theory $\longrightarrow$ non-relativistic quantum mechanics

weak interaction strengths between compounds,
saturation of forces, $\alpha \simeq 1/137$ *small* $\Rightarrow v \ll c$.

For some results, see [1].

(ii)
$$\begin{tikzcd}
\boxed{\text{non-relativistic quantum mechanics}} \arrow[dr, "\textit{many particles with weak interactions}"'] & & \boxed{\text{Newtonian mechanics}} \\
& \boxed{\text{non-relativistic classical field theory}} \arrow[ur, "\textit{attractive interactions}"'] &
\end{tikzcd}$$

A simple example of a solution of problem (ii) is the *main subject* of these notes.

Warning: Since, in natural units, $c = 1,\ \hbar = 1,\ \ell_P = 1$, the problems formulated above *cannot* be solved by letting c^{-1} or $\hbar$ or ℓ_P tend to 0 !

(3) The passage from microscopic theories at short distance — and time scales to *effective theories* at large distance — and time scales (which, hopefully, are easier to analyze) necessitates a deeper and mathematically more precise understanding of *renormalization group methods*.

In these notes, we describe some recent results which provide an example of a solution of problem (2), (ii). We consider a system of very many non-relativistic bosons with very weak two-body interactions and exhibit a class of states with the property that the time evolution of expectation values of certain operators in these states is approximately described by classical Hamiltonian equations of motion, more specifically by the *non-linear Hartree equations*. We then sketch how certain solutions of the non-linear Hartree equations approach solutions of *Newtonian equations of motion* for point particles when the two-body forces are attractive at short distances. Details may be found in [2].

2. Large systems of non-relativistic bosons

In non-relativistic quantum mechanics, pure states are unit rays in a separable Hilbert space, $\mathscr{H}$, mixed states are density matrices on $\mathscr{H}$. A specific physical situation is encoded in the choice of some concrete *algebra $\mathscr{A}$ of bounded operators contained in (or equal to) the algebra $B(\mathscr{H})$ of all bounded operators on $\mathscr{H}$. The time-evolution of an operator $a \in \mathscr{A}$ in the Heisenberg picture is given by

$$\mathscr{A} \ni a \mapsto a(t) := e^{i\widehat{H}t/\hbar}\, a\, e^{-i\widehat{H}t/\hbar} , \tag{1}$$

where $\widehat{H}$ is a selfadjoint operator densely defined on $\mathscr{H}$ (whose spectrum is usually assumed to be bounded from below).

As an example, we consider a system of N spinless, non-relativistic, identical quantum mechanical (point) particles in physical space $\mathbb{E}^3$ moving under the influence of an external force with potential W and of two-body interactions with potential $-\Phi$. As an algebra $\mathscr{A}$ we may, e.g., choose the algebra of smooth, bounded functions $a(x_1,\dots,x_N)$ on $\mathbb{R}^{3N}$ which are totally symmetric in their N arguments. Its spectrum corresponds to the space of configurations of N identical point particles.

The Hilbert space of state vectors $\mathscr{H} = \mathscr{H}_\sigma^{(N)}$ is chosen to be a subspace of the space $L^2(\mathbb{R}^{3N}, \Pi_{j=1}^N\, d^3x_j)$ of square-integrable functions on $\mathbb{R}^{3N}$ of a specific symmetry type σ under permutations of their N arguments ("quantum statistics"); i.e., a function $\psi \in \mathscr{H}_\sigma^{(N)}$ transforms under an irreducible representation σ of the group of permutations of $\{1,\dots,N\}$ when its arguments are permuted. When σ is the trivial representation ψ is totally symmetric in its N arguments, and we speak of *Bose–Einstein statistics*; when σ is the alternating representation ψ is totally anti-symmetric in its N arguments, and we speak of *Fermi–Dirac statistics*. (Higher-dimensional representations σ are sometimes called parastatistics.)

The Hamiltonian of the system is given by

$$\widehat{H} \equiv H^{(N)} := \sum_{j=1}^{N}\Big(-\frac{\hbar^2}{2}\triangle_j + W(x_j)\Big) - \sum_{1\le i<j\le N}\Phi(x_i - x_j) , \tag{2}$$

and we have chosen units so that the mass of a particle is equal to 1.

In Equation (2), $\triangle_j = \sum_{a=1}^3 \partial^2/(\partial x_j^a)^2$ and $x_j = (x_j^1, x_j^2, x_j^3)$ denotes the position of the j^{th} particle in $\mathbb{E}^3$ (in a fixed system of Cartesian coordinates). If W is e.g. a smooth positive function on $\mathbb{E}^3$ and Φ is "small" relative to $-\triangle$, in the sense of Kato, then $H^{(N)}$ is essentially selfadjoint on a natural domain dense in $L^2(\mathbb{R}^{3N}, \Pi\, d^3x_j)$. Since $H^{(N)}$ is symmetric under permutations of the particle labels $1,\dots,N$, the time evolution, $\exp(-iH^{(N)}t/\hbar)$, leaves the subspaces $\mathscr{H}_\sigma^{(N)}$ of $L^2(\mathbb{R}^{3N}, \Pi\, d^3x_j)$ invariant, for arbitrary σ.

There are straightforward generalizations of this class of systems to systems of several species of identical particles some of which may have non-zero quantum mechanical spin, e.g., to Coulomb system; see [3].

Two important problems in the analysis of such systems are (see [3]):

(A) *Stability* (i.e., the energy per particle is bounded from below by a constant $-\varepsilon$, uniformly in $N \Leftrightarrow H^{(N)} \ge -\varepsilon N, \forall N$); and

(B) *Existence of thermodynamic limit* (choose $W = W_\Lambda$ so as to confine the particles to a bounded region $\Lambda \subset \mathbb{E}^3$; keep the particle density $\rho := N/|\Lambda|$ fixed, where $|\Lambda|$

is the volume of Λ, and try to pass to the limit $\Lambda \nearrow \mathbb{E}^3$. — A necessary condition for the existence of a thermodynamic limit is stability.)

Much of *theoretical condensed matter physics* is the study of large systems of identical non-relativistic quantum mechanical point particles for which (A) and (B) hold. Such systems exhibit fascinating physical phenomena such as *Bose–Einstein condensation* (σ = trivial representation, two-body interactions repulsive); *superconductivity, Landau-* and *marginal Fermi liquids, Hall liquids, different forms of magnetism*, ... (σ = alternating representation). Precise mathematical understanding of some of these phenomena is only beginning to emerge; see e.g. [4] (and [5] for a review).

The topic of these notes is a study of dilute systems of a large number of neutral atoms with Bose–Einstein statistics (σ = trivial rep.) and with weak two-body interactions. If, in the initial state, the mean distance between atoms is sufficiently large and the average kinetic energy per atom is large then one may argue that, on sufficiently short time scales, short-range repulsion between the atoms can be neglected. Then the system can be described by a Hamiltonian $H^{(N)}$ of the form (2), where $-\Phi$ is e.g. the potential of a long-range attractive force. In this idealization, stability (A) is, however, usually violated.

We propose to identify a class of initial states for such systems with the property that the time evolution of the expectation value of certain operators in such states approaches one described by some classical, non-relativistic Hamiltonian PDE, in the limit where the strength κ of the two-body interaction tends to 0, with $N \propto \kappa^{-1}$.

In order to analyze such systems, it is convenient (though dispensable) to make use of the formalism of "second quantization". We imagine that the number N of atoms may fluctuate (e.g., because the system is coupled to a reservoir of atoms not included in our description). It is then convenient to introduce the Hilbert space

$$\mathscr{F} = \bigoplus_{N=0}^{\infty} \mathscr{H}^{(N)} \quad \mathscr{H}^{(0)} = \mathbb{C} , \tag{3}$$

where $\mathscr{H}^{(N)} = \mathscr{H}^{(N)}_{\sigma=\text{trival rep.}}$, which is commonly called *Fock space*. A vector $\underline{\psi} \in \mathscr{F}$ is a sequence

$$\underline{\psi} = \left\{ \psi^{(N)} \mid \psi^{(N)} \in \mathscr{H}^{(N)} \right\}_{N=0}^{\infty} \tag{4}$$

with

$$\| \underline{\psi} \|^2 := \sum_{N=0}^{\infty} \| \psi^{(N)} \|_2^2 < \infty .$$

The scalar product of two vectors $\underline{\psi}$ and $\underline{\varphi}$ is given by

$$\langle \underline{\psi}, \underline{\varphi} \rangle := \sum_{N=0}^{\infty} \left(\psi^{(N)}, \varphi^{(N)} \right) , \tag{5}$$

where $(\cdot,\cdot)$ is the usual L^2 scalar product. Let f be a test function on $\mathbb{E}^3$. We define an *"annihilation operator"* $a(f)$ on $\mathscr{F}$ by setting

$$a(f)\,\underline{\psi} \;=\; \underline{\psi}_f \;,$$

where

$$\psi_f^{(N)}(x_1,\ldots,x_N) \;:=\; \sqrt{N+1}\int d^3x\,\overline{f(x)}\;\psi^{(N+1)}(x,x_1,\ldots,x_N)\;. \tag{6}$$

The operator $a(f)$ is unbounded, but closable. The *"creation operator"* $a^*(f)$ is defined to be the adjoint of $a(f)$ on $\mathscr{F}$. It is an unbounded closable operator. It is easy to verify that

$$\begin{aligned} [a(f),a(g)] \;&=\; [a^*(f),a^*(g)] \;=\; 0\;,\\ [a(f),a^*(g)] \;&=\; (f,g)\;\mathbb{1}\;, \end{aligned} \tag{7}$$

for arbitrary test functions f and g. Equations (7) are called *canonical commutation relations*. The Hamiltonian $\widehat{H}$ on Fock space is given by

$$\widehat{H} \;=\; \bigoplus_{N=0}^{\infty} H^{(N)}\;,\quad \text{with } H^{(0)} \;=\; 0\;.$$

In terms of annihilation- and creation operators, $\widehat{H}$ can be expressed as follows:

$$\begin{aligned} \widehat{H} =& \frac{1}{2}\int d^3x\,[(\nabla a^*)(x)(\nabla a)(x) \,+\, W(x)\,a^*(x)\,a(x)]\\ &-\frac{1}{2}\int d^3x\int d^3y\,a^*(x)\,a^*(y)\,\Phi(x-y)\,a(y)\,a(x)\;, \end{aligned} \tag{8}$$

and we now use units such that $\hbar = 1$. The two-body potential $-\Phi$ is chosen as follows:

$$\Phi \;=\; \kappa\Phi_c\;,\quad \kappa \ll 1\;, \tag{9}$$

where $\Phi_c \in L^{\frac{3}{2}} + L^\infty$ (with $L^p = L^p(\mathbb{R}^3, d^3x)$); (depending on the analytical methods employed, one may need to also impose some regularity properties on first and second derivatives of Φ; see e.g. [6]). An example for Φ_c is

$$\Phi_c(x) \;\simeq\; |x|^{-6} + g|x|^{-1}\;,\quad g \ll 1, \tag{10}$$

for $|x|$ large compared to the diameter of an atom, and $\Phi_c(x)$ is regular near $x = 0$. The first term in Φ_c describes van der Waals attraction, the second term gravitational attraction between atoms. The external potential W is assumed to be a smooth positive function.

It is easy to check that

$$H^{(N)} \;\geq\; -C\,\kappa N^2\;, \tag{11}$$

for some finite constant C. For $N \propto \kappa^{-1}$, kinetic and potential energy terms in $H^{(N)}$ both scale like κ^{-1}.

Next, we introduce rescaled annihilation- and creation operators:

$$A_\kappa(f,t) \;:=\; \kappa^{1/2}\, e^{i\widehat{H}t}\, a(f)\, e^{-i\widehat{H}t} \tag{12}$$

($\hbar = 1$!), and

$$A_\kappa^*(f,t) \;:=\; (A_\kappa(f,t))^* \;. \tag{13}$$

Let $\underline{\varphi}$ be a vector in Fock space $\mathscr{F}$ with a finite number of particles and smooth k-particle wave functions of compact support, for all k. We define a vector $\underline{\theta}_\kappa$ by setting

$$\underline{\theta}_\kappa \;:=\; C_\kappa \left(a^*(\psi_0)\right)^{N_\kappa}\; \underline{\varphi}\;, \tag{14}$$

where ψ_0 is a smooth function of compact support which, for convenience, we choose to have $\| \psi_0 \|_2 = 1$,

$$N_\kappa \;=\; \left[\kappa^{-1}\right]\;, \tag{15}$$

where $[a]$ denotes the integer part of a positive number a, and the constant C_κ is chosen such that $\langle \underline{\theta}_\kappa, \underline{\theta}_\kappa \rangle = 1$.

Let $\psi(x,t)$ be a solution of the *non-linear Hartree equation*

$$i\partial_t \psi \;=\; -\frac{1}{2}\triangle\psi + W\psi - \left(\Phi_c * |\psi|^2\right)\psi \tag{16}$$

with initial condition

$$\psi(x,0) \;=\; \psi_0(x)\;. \tag{17}$$

We define

$$\psi(f,t) \;:=\; \int d^3x\, \overline{f(x)}\; \psi(x,t)\;,$$

and

$$\psi^*(f,t) \;:=\; \overline{\psi(f,t)}\;,$$

where f is a test function.

The following theorem is proven in [6].

Theorem 2.1 *Under the hypotheses described above,*

$$\lim_{\kappa\to 0} \langle \underline{\theta}_\kappa, \prod_{j=1}^{m} A_\kappa^*(f_j,t_j)\, A_\kappa(g_j,s_j)\, \underline{\theta}_\kappa \rangle = \prod_{j=1}^{m} \psi^*(f_j,t_j)\, \psi(g_j,s_j)\;, \tag{18}$$

for arbitrary $m = 1,2,\ldots$, arbitrary test functions $f_1,\ldots,f_m$, $g_1,\ldots,g_m$ and finite times $t_1,\ldots,t_m$, $s_1,\ldots,s_m$.

Thus, a classical limit described by the non-linear Hartree equation (16) is approached in systems of $N \sim \kappa^{-1}$ bosons interacting through two-body forces of strength κ, as κ tends to 0, for an appropriate choice of the initial state of the system.

In the following, we show that the non-linear Hartree equation is an example of a Hamiltonian PDE and then explore a Newtonian point-particle limit of the non-linear Hartree equation, for two-body potentials which are *attractive* at short distances.

The theorem quoted above is but one example of a result on the approach of quantum dynamics towards some classical Hamiltonian dynamics in a suitable limit. Another example would be a quantum spin system whose dynamics is expected to approach the one described by the Landau–Lifshitz equation in the limit where the local magnetization becomes large.

An unsatisfactory aspect of results of this type is that one must choose rather special sequences of states, $\{\underline{\theta}_\kappa\}$, in order to approach a classical limit. States leading to a classical limit do *not* form a linear space (which may explain why there are no puzzles related to the superposition principle). We do not understand much, yet, about a general class of states leading to classical limits, and in which physical situations such states appear naturally.

The material in the following sections is motivated by the above theorem, Equation (18): We study the NL Hartree equation (16) and the question under what circumstances it reduces to the Newtonian mechanics of point particles. We begin with a brief review of the *Hamiltonian nature* of the *non-linear Hartree equations*.

3. NL Hartree equations as a Hamiltonian system

The phase space for the non-linear Hartree equation (16) is the energy (Sobolev) space

$$\Gamma = H^1\left(\mathbb{R}^3\right) \tag{19}$$

with complex coordinates $\psi(x),\ \bar{\psi}(x)$. The symplectic two-form is given by $\frac{i}{2}\, d\psi \wedge d\bar{\psi}$. It leads to the following Poisson brackets

$$\begin{aligned} \{\psi(x),\ \psi(y)\} \;=\; \{\bar{\psi}(x),\ \bar{\psi}(y)\} \;=\; 0 \\ \{\psi(x),\ \bar{\psi}(y)\} \;=\; 2i\,\delta(x-y)\ . \end{aligned} \tag{20}$$

The Hamilton functional $\mathscr{H}$ leading to the NL Hartree equations (16) is given by

$$\mathscr{H}(\bar{\psi},\psi) \;=\; \frac{1}{4}\int \left[|\nabla\psi|^2 + 2W|\psi|^2 - \left(\Phi_c * |\psi|^2\right)|\psi|^2\right]\ , \tag{21}$$

with $\psi = \psi(x)$, $\int(\cdot) = \int_{\mathbb{R}^3} d^3x(\cdot)$, and $*$ denotes convolution. For $\Phi_c \in L^{\frac{3}{2}} + L^\infty$, $\mathscr{H}$ is well-defined on Γ (Sobolev- and Hölder inequalities), and it is bounded below on the spheres

$$\mathscr{S}_N \;:=\; \{\psi \mid \psi \in \Gamma,\ \mathscr{N}(\bar{\psi},\psi) \;=\; N < \infty\} \tag{22}$$

in phase space Γ, where

$$\mathscr{N}(\bar{\psi},\psi) \;:=\; \int |\psi|^2\ ; \tag{23}$$

see e.g. [7]. Hamilton's equations of motion for ψ are

$$\dot{\psi}(x,t) \;=\; \{\mathscr{H}(\bar{\psi},\psi)\,,\;\psi\}\;(x,t) \tag{24}$$

and are easily seen to be equivalent to the NL Hartree equation (16). From the form of $\mathscr{H}$ we infer the following *symmetries* and corresponding *conservation laws*.

(1) Gauge invariance of the first kind:

$$\psi(x)\;\mapsto\;e^{i\theta}\,\psi(x)\,,\quad \bar{\psi}(x)\;\mapsto\;e^{-i\theta}\,\bar{\psi}(x) \tag{25}$$

leaves $\mathscr{H}$ invariant; (25) is a symplectic flow generated by the Hamiltonian vector field associated with the functional $\frac{1}{2}\,\mathscr{N}(\bar{\psi},\psi)$. Thus $\mathscr{N}(\bar{\psi},\psi)$ must be conserved by the time evolution generated by (the Hamiltonian vector field determined by) $\mathscr{H}$, which means that

$$\{\mathscr{H},\mathscr{N}\}\;=\;0\,. \tag{26}$$

It follows that the spheres $\mathscr{S}_N$ defined in (22) are *invariant* under the time evolution.

(2) If $W=0$ and if Φ_c is rotation-invariant then arbitrary Galilei transformations are symmetries of $\mathscr{H}$. Space translations are generated by the momentum functional

$$\mathscr{P}(\bar{\psi},\,\psi)\;:=\;\frac{i}{2}\int\bar{\psi}\,\nabla\,\psi\,, \tag{27}$$

and rotations by the angular momentum functional

$$\mathscr{L}(\bar{\psi},\psi)\;:=\;\frac{i}{2}\int\bar{\psi}(x\wedge\nabla)\;\psi\,. \tag{28}$$

All components of $\mathscr{P}$ and $\mathscr{L}$ Poisson commute with $\mathscr{H}$. Velocity transformations (boosts), i.e. $x\mapsto x-vt$, are represented on time-dependent trajectories, $\psi(x,t)$, in Γ by

$$\psi(x,t)\;\mapsto\;\psi\,(v;x,t)\;:=\;\psi\,(x-vt,t)\;e^{i(v\cdot x-\frac{v^2}{2}t)}\,. \tag{29}$$

These transformations map solutions of the equations of motion (24) to other solutions of (24). It follows that the "center of mass motion" of a solution $\psi(x,t)$ of (24) is inertial.

Instead of the Hamiltonian formalism, we may make use of the *Lagrangian formalism* to study the Hartree equations (16). These equations are then obtained as the Euler–Lagrange equations corresponding to the *action functional*

$$S(\bar{\psi},\psi)\;=\;\int_{t_1}^{t_2}dt\;\Big[\frac{i}{2}\int\bar{\psi}\,(\cdot,t)\;\frac{\partial}{\partial t}\;\psi\,(\cdot,t)-\;\mathscr{H}\;\big(\bar{\psi}\,(\cdot,t)\,,\;\psi\,(\cdot,t)\big)\Big]\,, \tag{30}$$

by variation with respect to $\bar{\psi}$, (with $\delta\,\bar{\psi}(\cdot,t_i)=0$, for $i=1,2$).

Existence and regularity of global solutions of the Cauchy problem associated with the non-linear Hartree equation, under the conditions on Φ_c described above, is known. If $-\Phi_c$ is radially symmetric, decreasing (*repulsive* two-body forces) and of sufficiently short range then the scattering map associated with the non-linear Hartree equations exists and satisfies asymptotic completeness. These results are reviewed in [7]. In the situation of interest in these notes ($-\Phi_c$ radially symmetric, but *increasing*, i.e., for *attractive* two-body forces) existence and regularity are known from the results reviewed in [7], but the scattering theory is much more subtle, and only very preliminary results are available. Our main interest is in the Newtonian point-particle limit of the NL Hartree equations, for two-body forces which, at small distances, are *attractive*.

4. The point-particle limit of the NL Hartree equations with attractive two-body forces

For reasons that will become apparent shortly, we start by trying to find (local and absolute) minima of the Hamilton functional $\mathscr{H}$ restricted to a sphere $\mathscr{S}_N$, as defined in (22), for a vanishing external potential, $W = 0$. In this situation, the momentum- and angular momentum functionals, $\mathscr{P}$ and $\mathscr{L}$, are conserved. We should therefore study the (generalized) energy functional

$$\begin{aligned} \mathscr{E}(\bar{\psi},\psi;\nu,\pi,\lambda) \ :=\ & \mathscr{H}(\bar{\psi},\psi) + \frac{\nu}{2}\,(N-\mathscr{N}(\bar{\psi},\psi)) \\ & + \pi\cdot(P-\mathscr{P}(\bar{\psi},\psi)) + \lambda\cdot(L-\mathscr{L}(\bar{\psi},\psi))\ , \end{aligned} \tag{31}$$

where ν, π and λ are Lagrange multipliers. Variation with respect to $\psi, \bar{\psi}, \nu, \pi$ and λ yields the following variational equations:

$$-\frac{1}{2}\triangle\psi - \left(\Phi_c * |\psi|^2\right)\psi - \nu\psi - i\pi\cdot\nabla\psi - i\lambda\cdot(x\wedge\nabla)\,\psi \;=\; 0 \tag{32}$$

as well as the complex conjugate equation, and

$$\mathscr{N}(\bar{\psi},\psi) = N\,, \quad \mathscr{P}(\bar{\psi},\psi) = P\,, \quad \mathscr{L}(\bar{\psi},\psi) = L\,. \tag{33}$$

We do not know much about the general solutions to these equations. But, for the purposes of these notes, the following special case is particularly important: We search for an absolute minimum, Q_N, of $\mathscr{H}(\bar{\psi},\psi)\big|_{\mathscr{S}_N}$ which is rotation-invariant and has zero momentum. The function Q_N is the solution of the equations

$$\begin{aligned} -\frac{1}{2}\triangle\psi - \left(\Phi_c * |\psi|^2\right)\psi &= \nu\,\psi\,, \\ \mathscr{N}(\bar{\psi},\psi) &= N\,, \end{aligned} \tag{34}$$

and we henceforth set $\nu =: E$. It follows that

$$E \;=\; \frac{1}{2N}\int \left[|\nabla Q_N|^2 - \left(\Phi_c * |Q_N|^2\right)|Q_N|^2\right]\ , \tag{35}$$

which is strictly *negative*, for a non-trivial minimum Q_N.

Fairly standard methods of variational calculus show that there exists some finite $N_* = N_*(\Phi_c)$ such that, for $N > N_*$, Equations (34) have a non-trivial, smooth, positive solution $Q_N(x)$ which decays exponentially in $|x|$, with decay rate $\sqrt{-E}$. From the theory of binding in Schrödinger quantum mechanics one infers that $N_*(\Phi_c) = 0$, if $\Phi_c(x)$ is positive and decreases in $|x|$ more slowly than $|x|^{-2}$; but $N_*(\Phi_c) > 0$ if Φ_c is of short range. Covariance under translations and velocity transformations then implies that

$$\psi_N(v,a;x,t) \;:=\; Q_N(x-a-vt)\; e^{i\left(v\cdot x-\left[\frac{v^2}{2}+E\right]t\right)} \tag{36}$$

solves the non-linear Hartree equations (16), for an arbitrary velocity $v \in \mathbb{R}^3$. It describes a *"soliton"* traveling with velocity v.

Let $\mathscr{H}''$ denote the Hessian of $\mathscr{H}\big|_{\mathscr{S}_N}$ at Q_N. Then one finds that

$$\left(Q_N, \mathscr{H}''\, Q_N\right) \;=\; \varepsilon_0\; (Q_N, Q_N)\,, \quad \varepsilon_0 \;<\; 0\,. \tag{37}$$

In fact, $\mathscr{H}''$ has precisely one eigenvector ϕ_0 corresponding to a negative eigenvalue. Furthermore,

$$\mathscr{H}''\; \frac{\partial}{\partial x^a}\, Q_N \;=\; 0\,, \;\text{ for }\; a \,=\, 1,2,3, \tag{38}$$

which follows from the translation invariance of $\mathscr{H}$, and the continuous spectrum of $\mathscr{H}''$ covers the interval $[-E, \infty)$, with $-E > 0$.

Assumption $*$ It will be assumed henceforth that Φ_c can be chosen such that the multiplicity of the eigenvalue $\varepsilon_1 = 0$ of $\mathscr{H}''$ is equal to 3.

The eigenspace of $\mathscr{H}''$ corresponding to the eigenvalue 0 is then spanned by the vectors $\frac{\partial}{\partial x^1} Q_N$, $\frac{\partial}{\partial x^2} Q_N$, $\frac{\partial}{\partial x^3} Q_N$, and it follows that

$$\left(\phi, \mathscr{H}''\phi\right) \;\geq\; \varepsilon_2\, (\phi, \phi)\;, \quad 0 < \varepsilon_2 \leq -E\;, \tag{39}$$

for arbitrary $\phi \in L^2(\mathbb{R}^3)$, with $\phi \perp Q_N$, $\frac{\partial}{\partial x^a} Q_N$, $a = 1,2,3$.

We are now prepared to discuss the Newtonian point-particle limit of the non-linear Hartree equation. Our discussion is heuristic; for mathematical results see [2].

We choose an external potential W of the form

$$W(x) \;\equiv\; W^{(\varepsilon)}(x) \;:=\; V(\varepsilon x)\;,$$

where V is a positive, smooth function on $\mathbb{R}^3$, and $\varepsilon \ll 1$ is a parameter. Furthermore, the two-body potential $-\Phi_c$ is chosen to be

$$\Phi_c(x) \;=\; \Phi_s(x) + \Phi_\ell(\varepsilon x)\;, \tag{40}$$

where $\Phi_s(x)$ is a rotation-invariant, smooth function decaying rapidly in $r := |x|$, as $r \to \infty$, and with the properties that

$$\frac{\partial \Phi_s(r)}{\partial r} < 0 , \quad \text{for } r > 0 , \tag{41}$$

and that Assumption $*$ above holds for $\Phi_c = \Phi_s$. The potential Φ_ℓ is rotationally invariant and may be of long range, e.g.,

$$|\Phi_\ell(x)| \sim r^{-1} , \quad \text{as } r \to \infty .$$

For technical convenience, we also assume that Φ_ℓ is once continuously differentiable, with $|\partial\Phi_\ell/\partial r|$ uniformly bounded in r.

Next, we pick a positive integer k and k positive numbers $N_1, \dots, N_k$, with $N_j > N_*(\Phi_s)$, for all j. For $\varepsilon = 0$ and $N > N_*(\Phi_s)$, we define

$$\delta_N := \sqrt{N^{-1} \int d^3x\, Q_N(x)^2 x^2} . \tag{42}$$

We consider a configuration of k solitons $Q_{N_j}(x - q_j)$, $q_j \in \mathbb{R}^3$, $j = 1, \dots, k$, with the following properties: Each $Q_{N_j}(x)$ is a solution of equations (34), with $N = N_j$, for $\Phi_c = \Phi_s + \Phi_\ell(0)$, i.e., $\varepsilon = 0$; and

$$\big(\max_{j=1,\dots,k} \delta_{N_j} \big) / \big(\min_{1 \le i < j \le k} |q_i - q_j| \big) \le \varepsilon . \tag{43}$$

Our goal is to construct a solution ψ_ε of the non-linear Hartree equation (16) of the form

$$\psi_\varepsilon(x,t) = \sum_{j=1}^{k} Q_{N_j}(x - q_j(t))\, e^{i\theta_j(x,t)} + h_\varepsilon(x,t) , \tag{44}$$

where $q_j(0) = q_j$, $\dot{q}_j(0) = v_j$, $j = 1, \dots, k$, with the following properties: There is a positive constant T such that, for all times t with $|t| < \frac{T}{\varepsilon}$,

$$\begin{aligned} &\text{(i)} \quad \| \mathrm{h}_\varepsilon(\cdot,\mathrm{t}) \|_{\mathrm{H}^1} = \mathrm{o}(\varepsilon) , \\ &\text{(ii)} \quad \theta_{\mathrm{j}}(\mathrm{x},\mathrm{t}) = \dot{\mathrm{q}}_{\mathrm{j}}(\mathrm{t}) \cdot \big[\mathrm{x} - \mathrm{q}_{\mathrm{j}}(\mathrm{t})\big] + \vartheta_{\mathrm{j}}(\mathrm{t}) , \end{aligned}$$

where $\vartheta_j(t)$ is independent of x; the trajectories $q_1(t), \dots, q_k(t)$ and the phases $\vartheta_1(t), \dots, \vartheta_k(t)$ will turn out to be determined by the non-linear Hartree equations (16) and properties (i) and (ii).

In order to convince ourselves that the ansatz (44) with properties (i) and (ii) is plausible, we evaluate the action functional $S(\bar{\psi}, \psi)$ introduced in Equation (30) on the ansatz functions $(\bar{\psi}, \psi) = (\bar{\psi}_\varepsilon, \psi_\varepsilon)$, with ψ_ε as in (44). We shall regard the soliton trajectories $q_1(t), \dots, q_k(t)$, the phases $\vartheta_1(t), \dots, \vartheta_k(t)$, and the small amplitude wave h_ε as variational parameters of the ansatz $(\bar{\psi}_\varepsilon, \psi_\varepsilon)$. After a moderately lengthy calculation one finds that, for a certain choice of $\dot{\vartheta}_j(t)$,

$$\begin{aligned} S(\bar{\psi}_\varepsilon, \psi_\varepsilon) = \int_{-\tau}^{\tau} dt \sum_{j=1}^{k} \Big[& \frac{N_j}{2}\, \dot{q}_j(t)^2 - N_j V(\varepsilon q_j(t)) \\ & + \sum_{i: i<j} N_i N_j \Phi_\ell(\varepsilon(q_i(t) - q_j(t))) + o(\varepsilon) \Big] \end{aligned} \tag{45}$$

for $\tau < \frac{T}{\varepsilon}$. Up to error terms $\sim o(\varepsilon)$, which are the source of a variety of mathematical subtleties, this is the action for a system of k Newtonian point particles with masses $N_1, \dots, N_k$ moving under the influence of an external acceleration field with potential $W^{(\varepsilon)}$ and of two-body forces with potential $-N_i N_j \Phi_\ell(\varepsilon(q_i - q_j))$, $1 \le i < j \le k$; $q_j(t)$ is the position of the j^{th} particle at time t.

Expression (45) for $S(\bar{\psi}_\varepsilon, \psi_\varepsilon)$ suggests that, for $S(\bar{\psi}, \psi)$ to have a critical point at $(\bar{\psi}, \psi) = (\bar{\psi}_\varepsilon, \psi_\varepsilon)$, with ψ_ε given by (41) and satisfying properties (i) and (ii), the particle trajectories $\{q_j(t)\}_{j=1}^{k}$ must be solutions of Newton's equations of motion

$$\ddot{q}_j(t) = -\varepsilon \left[\nabla V(\varepsilon q_j(t)) - \sum_{i \neq j} N_i \nabla \Phi_\ell(\varepsilon(q_i(t) - q_j(t))) \right] + a_j(t)\,, \tag{46}$$

where $j = 1, \dots, k$, and the *"friction force"* $a_j(t)$ satisfies a bound $|a_j(t)| = o(\varepsilon)$, for $|t| < \frac{T}{\varepsilon}$.

These ideas are made precise (in the form of mathematical theorems) in [2], using methods partly based on the work of Weinstein [8], for just one soliton in an external potential $W^{(\varepsilon)}$. But the methods in [2] can be extended to general k.

Apparently, we have gained insight into how Newtonian point-particle mechanics with small friction forces can emerge from the non-linear Hartree equation with *attractive* two-body forces of short range (Φ_s) and weak attractive *or* repulsive two-body forces of very long range $(\Phi_\ell(\varepsilon\,\cdot))$ by considering the evolution of configurations of far-separated solitons over large, finite intervals of time. The friction forces $(a_j(t))$ appearing in Newton's equations of motion originate in the emission of small-amplitude, dispersive radiation from the solitons. This is an example of a general and quite fundamental phenomenon: *friction* (or dissipation) through *emission of radiation* in *conservative* (classical and quantum mechanical) *systems* of infinitely many degrees of freedom.

For similar considerations in the context of vortex dynamics in a Ginzburg–Landau superfluid see [9].

The results discussed above appear to be a special case of more general results on the Newtonian limit of the non-linear Hartree equation. One might imagine that it is possible to construct *"rotating-body"* solutions of the non-linear Hartree equations with non-zero angular momentum relative to their center of mass. Such solutions are, in general, unstable. Nevertheless, one could attempt to construct solutions of the non-linear Hartree equation which, over a large finite interval of time, describe a configuration of finitely many rotating bodies, whose motion is described by a system of Euler-type equations with small friction terms, emitting small-amplitude dispersive radiation.

The results reviewed in Equations (39) through (46) and the speculations just described raise the issue of *asymptotic properties* of the dynamics determined by the non-linear Hartree equation in the limit, as time tends to $\pm\infty$. Such problems belong to the realm of non-linear *scattering theory*. In [2], a result on the scattering of small-amplitude waves of a single soliton has been established. It requires $W(x)$ and $\Phi_c(x)$ to be smooth and of short range. We consider an "asymptotic profile" given by

$$\psi_{as}(x,t) \;=\; Q_N(x-vt)\, e^{i(x\cdot v\,-\,[\frac{v^2}{2}+E]t)} \;+\; h(x,t) \;, \tag{47}$$

where h is a solution of the free-particle Schrödinger equation

$$i\,\partial_t\, h(x,t) \;=\; -\,\frac{1}{2}\,\triangle\, h(x,t)\;,$$

with $h(x,0)\in H^3(\mathbb{R}^3)\cap W^{3,1}\left(\mathbb{R}^3,\left(1+|x|^2\right)d^3x\right)$, and $\hat{h}(v,0)=0$. The claim is that there are solutions, $\psi_\pm(x,t)$, of the non-linear Hartree equation (16) such that

$$\psi_\pm(x,t) \underset{t\to+\infty}{\longrightarrow} \psi_{as}(x,t) \tag{48}$$

in $H^1(\mathbb{R}^3)$.

Thus, (non-linear) *Møller wave maps* $\Omega_\pm$ exist (as symplectic maps) on asymptotic profiles of the form (47); (see also [7] for background material on non-linear scattering theory). Of course, the results described here do not bring us anywhere close to an understanding of asymptotic completeness of the scattering map.

5. More about open problems, conclusions

In this last section, we draw the reader's attention to some interesting open problems.

(1) Clearly, a deeper understanding of the non-linear scattering theory of solitons and waves for the non-linear Hartree equation would be highly desirable. In particular, it would be important to gain more detailed insight into the domain of definition and the *image* of the Møller wave maps $\Omega_\pm$.

A comparatively simple situation has been studied by Soffer and Weinstein [10]. They consider a smooth external potential W of short range with exactly one quantum mechanical bound state, i.e., the spectrum of the operator $-\frac{1}{2}\triangle+W$ consists of one simple eigenvalue $\varepsilon<0$ and of purely absolutely continuous spectrum covering $[0,\infty)$. One must also assume that there is no zero-energy resonance. They consider a local non-linearity (NL Schrödinger equation); but their techniques can be extended to the NL Hartree equation with Φ_c of short range. They construct small-amplitude non-linear bound states (stationary solutions of (16)) by standard bifurcation theory techniques. They then exhibit a class of initial conditions with the property that the asymptotic behavior of solutions of (16) with these initial conditions is that of a non-linear bound state plus a purely dispersive wave which tends to zero (pointwise) at the free dispersion rate, as $t \to \pm\infty$. They also show that initial conditions close to a (small-amplitude) non-linear bound state have this property.

Obviously, one would like to extend these results to external potentials W with more than one bound state and understand the radiative decay of initial conditions close to an *excited* boundstate of $-\frac{1}{2}\triangle + W$ to a non-linear ground state plus dispersive radiation. One would also like to go *beyond* results for small-amplitude initial conditions. In this case, it can happen that the restriction of the Hamilton functional $\mathscr{H}(\bar{\psi}, \psi)$ (see Equation (21)) of the non-linear Hartree equation (16) to a sphere $\mathscr{S}_N$ in phase space Γ (see (22)) has several distinct local quadratic minima, provided N is large enough; (choose W to have several minima separated by large barriers and $-\Phi_c$ attractive). One would then like to understand the shape of the *"basins of attraction"* in phase space of these local minima. [The forward (backward) basin of attraction of a one-parameter family of local minima of $\mathscr{H}\big|_{\mathscr{S}_N}$ parametrized by N consists of all initial conditions in phase space Γ which approach an element of this family plus dispersive radiation decaying to zero, as $t \to +\infty$ ($t \to -\infty$, respectively). More generally, one may introduce a notion of a *center manifold* of (asymptotically) attracting configurations of solitons (freely moving, for $W = 0$) to which solutions of the non-linear Hartree equation with initial conditions sufficiently close to the center manifold converge, as $t \to +\infty$, or $t \to -\infty$. In this connection, see e.g. [11].]

(2) Consider a configuration ψ_ε of, say, just two far-separated solitons with initial positions q_1, q_2 and initial velocities $v_1 = \dot{q}_1(0)$, $v_2 = \dot{q}_2(0)$, as described in Equation (44), with $h_\varepsilon(x,0) = 0$. Let us assume that the two-body force with potential $-\Phi_\ell$ is purely attractive and of short range. We choose the initial conditions, (N_1, q_1, v_1) and (N_2, q_2, v_2) in such a way that the two solitons form a bound system, in the sense that

$$\frac{N_1}{2}\, v_1^2 \,+\, \frac{N_2}{2}\, v_2^2 \,-\, N_1 N_2 \Phi_\ell\,(\varepsilon\,(q_1 - q_2)) \,<\, 0\,. \tag{49}$$

We would like to understand the fate of this configuration, as $t \to \infty$. To begin with, we would like to estimate the power $P_R(t)$ of dispersive radiation through a sphere of radius $R \gg \max\,(|q_1|, |q_2|)$; see [9] for some results on a related problem. Furthermore, we would like to show that a configuration of two bound solitons collapses to a single soliton moving through space with a constant velocity, for $W = 0$ (!), plus a dispersive outgoing wave tending to O (pointwise) at the free dispersion rate; ("radiative collapse of a binary system").

(3) It appears reasonable to imagine that if the potential Φ_ℓ is chosen to be given by

$$\Phi_\ell(x) \simeq |x|^{-1},$$

for $|x|$ large, (Φ_s as in Section 4 and $W=0$), the non-linear Hartree equation (16) can be used to describe Newtonian gravity of a giant cloud of bosonic atoms, with built-in dispersive friction. It would be interesting to understand how, on intermediate time scales, inhomogeneities in the initial conditions grow to form a structure consisting of rotating bodies plus dispersive radiation ("structure formation"), before the system collapses into a number of far separated solitons escaping from each other. Perhaps, one may gain some insight into such problems with the help of numerical simulations; see e.g. [12].

(4) It is of interest to study transport phenomena described by the non-linear Hartree equation with a *random* external potential W whose distribution is homogeneous and has correlations of short range. For some results in this direction see [13].

Perhaps most importantly, we would like to understand much more about how non-linear equations of classical physics emerge as descriptions of quantum systems in certain asymptotic regimes.

Progress in theoretical physics is achieved in many different ways. If one is very lucky (and ingenious) one may discover new Laws of Nature or *new* physical theories or new mathematical structure useful to formulate such theories. More modestly, one may attempt to improve the mathematical understanding of *known* physical theories or derive new consequences of such theories. It appears safe to predict that we will be sailing well into the 21$^{\text{st}}$ century with plenty of interesting questions about physical theories discovered during the past three hundred years to worry about, and that "analysis and physics" will be a worthy partner of the currently more popular "geometry and physics".

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