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Derivation and Meaning of the Newton-Schrödinger Equation

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Abstract

In this thesis, we provide a mathematically rigorous derivation of the Newton-Schrödinger equation as an effective equation for a system of identical bosons interacting via gravity in the Vlasov limit. Moreover, error estimates coming from a finite number of particles are given. We shortly give an overview of some possible generalizations of our proof. Furthermore, we critically discuss other contexts in which the Newton-Schrödinger equation appears in the literature.

Contents

1 Introduction

Establishing a mathematically well-defined and experimentally testable theory of quantum gravity is undoubtedly one of the (if not even the) greatest task of modern theoretical physics. The conceptual and mathematical difficulties by constructing such a theory are so grave that many of the best theoretical physicists were not able to do so despite greatest efforts and various different attempts.

One of the most difficult problems in formulating a theory of quantum gravity is that it is not clear at all how to quantize gravity. Since the gravitational force is rather weak, the theory of semiclassical gravity as a (probably effective) theory has been established in which one only quantizes the matter and treats the gravitational force classically. However, even this theory is very difficult to analyze. Hence one is forced to simplify it further.

The most natural description for a non-relativistic quantum mechanical system is a Schrödinger equation with a gravitational interaction potential

$$i\hbar \frac{\partial \psi(\mathbf{x},t)}{\partial t} = \left(-\sum_{i=1}^{N} \frac{\hbar^2}{2m_i} \Delta_i - Gm^2 \sum_{i \neq j} \frac{1}{|x_i - x_j|} \right) \psi(\mathbf{x},t). \tag{1.1}$$

For a many-body system, solving this partial differential equation becomes a very hard or even impossible task, too. Therefore one has to find a effective equation for such systems.

The Newton-Schrödinger equation

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 - Gm^2 \int d^3x' \frac{|\psi(x',t)|^2}{|x - x'|} \right) \psi(x,t) \tag{1.2}$$

has been considered to be the right effective equation for the mean field describing a system of infinitely many particles governed by (1.1). In this thesis we prove that this is indeed the case, at least for a system of identical bosons.

In this thesis, we will keep, for clarity, the physical constants most of the time.

In the subsequent section (section 2) we present the foundations of semiclassical gravity. Some heuristic arguments for semiclassical gravity following from general relativity are provided. Furthermore we discuss the major difficulties regarding semiclassical gravity shortly. After that we argue that equation (1.1) can be derived from semiclassical gravity by linearizing and taking the Newtonian limit of the latter.

Section 3 provides some arguments for eq. (1.1) not involving semiclassical gravity.

The focus of this thesis lies on section 4 in which our main result is proven. We provide a derivation of the Newton-Schrödinger equation as a mean-field equation from the many-body Schrödinger equation with Newtonian potential in the limit of infinitely many particles. For the case of a gas of identical bosons, this is done in all mathematical details using Grønwall's lemma. Furthermore, we provide estimates of errors coming from a finite number of particles. Afterwards we provide an overview of possible generalizations of that proof, e.g. for fermionic systems.

In section 5, we discuss the different roles that the Newton-Schrödinger equation plays in the literature critically.

In the last section (sec. 6) we summarize the most important results once again.

2 From Semiclassical Gravity to a Schrödinger Equation with a Gravitational Potential

Nobody knows how to formulate a theory of quantum gravity, i.e. a theory of quantum matter moving in a quantized gravitational field, which is mathematically well-defined and provides experimentally testable results. The canonical quantization of gravity yielding the Wheeler-DeWitt equation and the theory of loop quantum gravity are examples of attempts towards such a theory. However, they are full of mathematical and interpretational problems.

The root problem seems to be quantizing the gravitational field. Hence, it was proposed in [1, 2] not to quantize gravity but treat the gravitational fields classically. This theory is called semiclassical gravity.

Generally, the notion of semiclassical gravity refers to some kind of theory that regards matter as quantized field operators but treats the gravitational field "classically", i.e. not quantized. The motion of the matter fields is described by the so-called quantum field theory in curved space-time [3–5].

Whether this classical treatment of gravity is valid on a fundamental level or only for an effective theory is a widely discussed issue (cf. e.g. [6–8]). If one regards semiclassical gravity as an approximation to a full theory of quantum gravity, the regime in which it is fine as an effective theory is when the frequency of the quantized gravitation is very small compared with the Planck frequency[1], and in addition, the energy of particles created resp. annihilated by the quantum fluctuations is small compared with the one of the gravitational field (cf. e.g. [9, 10]).

In our opinion there is a strong evidence that the theory of semiclassical gravity is only an effective theory and not a fundamental one. Hence, we will assume in our derivation of the NSE that there is a fundamental theory of quantum gravity from which semiclassical gravity follows. Some arguments why we regard semiclassical gravity as effective theory will be discussed after deriving the Newton-Schrödinger equation, in sec. 5.

2.1 Semiclassical Einstein Equations

The purpose of semiclassical gravity is to take into account the most important backreaction from the quantum matter onto the classical background, i.e. the classical gravitational field of general relativity. To determine the part of the backreaction which contributes most one can use the method of the effective action. This method is also used in other quantum field theories for the same purpose. It is based on the path integral formulation. We will not explain it in all details since for this thesis the details are not important. (See [5, 11, 12] for more details)

The basic idea of the method of effective action is to transfer the principle of stationary action

[1] $\omega_p = \frac{c^5}{G\hbar} \approx 10^{43} s^{-1}$

from classical physics to quantum physics. Of course, one generally has to consider all possible paths in the full quantum case. However, due to a stationary phase argument the paths which contribute most are the ones whose action is approximately equal to the classical action. Hence considering those yields exactly the limiting case one is interested in. The effective action of a quantum system under an operator happens to be the expectation value of that operator since due to the path integral formulation the paths whose action is nearly the classical action are determined by the expectation value of the quantum operator. This can be seen by using the generating function belonging to that operator. As said before, the mathematical details of the effective action method are beyond the scope of this thesis.

The classical Einstein-Hilbert action of general relativity is

$$S_{EH} = \frac{c^4}{8\pi G} \int \sqrt{g} R d^4 x \tag{2.1}$$

where G is the Newtonian constant of gravity, c is the speed of light, g denotes the determinant of the metric and R is the Ricci scalar. In this thesis we use the convention (-,+,+,+) for the signature of the metric, and the other sign conventions are also adopted from [13].

In classical general relativity the vacuum Einstein field equations are derived by taking the functional derivative of that action with respect to the metric tensor $g_{\mu\nu}$ and applying the principle of the stationary action. In presence of matter one has to take into account the derivative of the coupled action of the matter, too. This term which arises due to matter/energy in the classical theory is (proportional to) the so-called energy-momentum-tensor.

Following the method of the effective action, this statement can be rewritten for quantum matter in terms of the expectation value of the quantized energy-momentum-tensor. This yields the semiclassical Einstein equations

$$G_{\mu\nu} := R_{\mu\nu} + \frac{1}{2} g_{\mu\nu} R = \frac{8\pi G}{c^4} \left\langle \hat{T}_{\mu\nu} \right\rangle_\phi \tag{2.2}$$

with $G_{\mu\nu}$ being the Einstein tensor, $R_{\mu\nu}$ the Riemann tensor, $g_{\mu\nu}$ the metric tensor and $\left\langle \hat{T}_{\mu\nu} \right\rangle_\phi$ the expectation value of the quantized energy-momentum-tensor of the general theory of relativity. The expectation value is to be taken with respect to some quantum field ϕ. This quantity can physically be interpreted as the mass density of the field.

Taking the expectation value of a quantum operator is also the most natural operation in order to get a real number. Since the components of $G_{\mu\nu}$ are no quantum operators but real numbers one has to get some real number out of the quantized energy-momentum-tensor. As explained before, the operation of taking the expectation value also follows from the method of the effective action.

2.2 Remarks on Difficulties of Semiclassical Gravity

One of the most (if not the most) severe difficulty of semiclassical gravity is the question how to quantize the energy-momentum-tensor. The problem thereby is that it is not renormalizable (cf. e.g. [4, 5, 14] and others). There have been different ways proposed how to pass that difficulty.

The unrenormalizability is much more grave than that of quantum electrodynamics.

In [14] the approximate energy-momentum-tensors for several different fields in a weak gravitational field are calculated by using Feynman diagrams up to one loop.

Wald ([4, 15] considers an axiomatic approach. He develops several axioms that the expectation value of quantized energy-momentum-tensor has to fulfil. From these axioms he constructs the expectation values of some quantized energy-momentum-tensors for simple systems.

There is however no mathematically well-defined method to construct the quantized energy-momentum-tensor in an unambiguous manner.

Moreover, another problematic aspect regarding the semiclassical Einstein equations is that in classical general relativity the Einstein tensor is conserved identically, i.e. $\nabla^{\mu} G_{\mu\nu} = 0$. However, this does not hold for the expectation value of the energy-momentum-tensor in general. Hence, the left hand side of eq. (2.2) is covariantly conserved while the right hand side is not. That fact is not that bad if one considers semiclassical gravity only as an effective theory since effective theories are only valid in a certain regime, and there the difference does not really matter. But if one regards semiclassical gravity as the fundamental theory for quantum matter moving through gravitational backgrounds (cf. sec. 5 for a further discussion) one has to deal with that incompatibility.

We mention for completeness that there have been proposed other approaches to take into account the backreaction of quantum matter onto a background metric, e.g. the so-called stochastic gravity (cf. [16]). In this theory a stochastic term is added to the effective action. This yields the Einstein-Langevin equation which is a stochastic extension of the semiclassical Einstein equations and which takes quantum fluctuations of the system into account as sources of gravity. In this thesis, we will not consider it further, since it does not yield a Newton-Schrödinger equation.

We also note that (as already the classical Einstein field equations) the semiclassical Einstein equations are nonlinear and hence very difficult to solve. In addition, the semiclassical Einstein equations are non-local due to the non-locality of the quantum field. This makes finding a solution notoriously difficult. Therefore some approximations of the semiclassical Einstein equations are needed.

In this thesis, we only regard the so-called Newtonian limit of semiclassical gravity.

2.3 Newtonian Limit of Semiclassical Gravity

We only provide a short and heuristic argumentation here (some more details can be found in [6, 7]). Assuming that semiclassical gravity is only an effective theory valid for small frequencies of the metric and small quantum fluctuations, one can linearize semiclassical gravity for a weak gravitational field around flat space-time. Therefore the line element of the metric is

$$ds^2 = -(1 - 2V)dt + dx \tag{2.3}$$

like in the weak field limit of classical general relativity. In this metric the semiclassical Einstein equation can be written as

$$-\Delta V = 4\pi G \langle \hat{T}_{00} \rangle_{\phi} \tag{2.4}$$

with Δ being the Laplacian and $\hat{T}_{00}$ the "time-time" component of the quantized energy-momentum-tensor. Taking only the "time-time" component corresponds to the non-relativistic limit. This is completely analogous to the classical case.

Solving Poisson's equation eq. (2.4) yields

$$V(\mathbf{x}) = -G \int_{\mathbb{R}^3} \frac{\langle \hat{T}_{00}(\mathbf{x}') \rangle_\phi}{|\mathbf{x} - \mathbf{x}'|}. \tag{2.5}$$

The dependence of $\hat{T}_{00}$ on the coordinate occurs because of constraints. After second quantization and mass renormalization this yields

$$i\hbar \frac{\partial \psi(\mathbf{x}, t)}{\partial t} = \left(-\sum_{i=1}^{N} \frac{\hbar^2}{2m_i} \Delta_i - Gm^2 \sum_{i \neq j} \frac{1}{|x_i - x_j|} \right) \psi(\mathbf{x}, t) \tag{2.6}$$

where ψ is the wave function of the particles coming from the second quantized field ϕ. This equation is the starting point of our derivation of the Newton-Schrödinger equation in sec. 4.

3 Remark on the Schrödinger Equation with a Gravitational Potential

There are also other ways to derive this equation. For example, in [7] this equation is also obtained by starting with the Einstein-Hilbert action of classical general relativity (2.1) with some coupled classical fields, e.g. a minimal coupled Klein-Gordon scalar field. To perform a reduced state space quantization one has to perform a 3+1 decomposition of the resulting action (see also [17] for a explanation of this method of decomposition of space-time into space-like hypersurfaces). For this decomposed action they perform the weak field limit by linearizing this action. This yields a Lagrangian and after a Legendre transformation a (still classical) Hamiltonian. Then after fixing the gauge and taking the non-relativistic limit the canonical quantization rules can be applied to obtain eq. (2.6). Since this is done in [7] in a mathematically rather rigorous manner, we do not recap the mathematical details of this derivation.

Of course, one can also guess this equation as it is. It is simply a Schrödinger equation with a Newtonian gravitational potential. In principle one does not need to derive it from general relativity or semiclassical gravity since it is the natural equation for non-relativistic quantum particles interacting via Newtonian gravitation.

4 Derivation of the Newton-Schrödinger Equation as a Mean Field Equation

In sec. 2 and 3 we provided some arguments why

$$i\hbar\frac{\partial\psi(\mathbf{x},t)}{\partial t} = \left(-\sum_{i=1}^{N}\frac{\hbar^2}{2m_i}\Delta_i - Gm^2\sum_{i\neq j}\frac{1}{|x_i - x_j|}\right)\psi(\mathbf{x},t)$$

correctly describes a non-relativistic quantum system with gravitational interaction potential.

Our purpose now is to show that the effective behavior of a quantum system evolving due to (2.6) is described by the Newton-Schrödinger equation (1.2) if the number of particles in the system is very large, i.e. in the limit $N \to \infty$.

Particularly, this holds if the kinetic energy is of the same order of magnitude as the potential energy[2]. However, the potential energy in (2.6) does not scale in the same way with N as the kinetic energy, since the sum contained in the potential is a double sum with $N(N-1)$ summands altogether, whereas the sum in the kinetic term has only N summands. To compensate this difference we have to scale it with an additional factor $(N-1)^{-1}$ which we insert manually in (2.6).

$$i\hbar\frac{\partial\psi(\mathbf{x},t)}{\partial t} = \left(-\sum_{i=1}^{N}\frac{\hbar^2}{2m_i}\Delta_i - (N-1)^{-1}Gm^2\sum_{i\neq j}\frac{1}{|x_i - x_j|}\right)\psi(\mathbf{x},t) \tag{4.1}$$

Of course, that solution seems to be very unphysical at first glance. However, one retains an equation that resembles (2.6) simply via scaling of the space and time coordinates.

Substituting $\mathbf{y} = (N-1)\mathbf{x}$ yields

$$i\hbar\frac{\partial\psi(\mathbf{y},t)}{\partial t} = \left(-(N-1)^{-2}\sum_{i=1}^{N}\frac{\hbar^2}{2m_i}\tilde{\Delta}_i - (N-1)^{-1}Gm^2\sum_{i\neq j}\frac{1}{(N-1)|y_i - y_j|}\right)\psi(\mathbf{y},t)$$

where $\tilde{\Delta}$ is the Laplacian in the new y-coordinates. Now we scale the time $\tau = (N-1)^2 t$ and receive

$$i\hbar\frac{\partial\psi(\mathbf{y},\tau)}{\partial\tau} = \left(-\sum_{i=1}^{N}\frac{\hbar^2}{2m_i}\tilde{\Delta}_i - Gm^2\sum_{i\neq j}\frac{1}{|y_i - y_j|}\right)\psi(\mathbf{y},\tau) \tag{4.2}$$

which has exactly the same form as (2.6) but in the new coordinates.

Let us shortly explain why the scalings are physically reasonable. The scaling of the spatial coordinates means nothing else but that the more particles are there the more space they need. That is, the volume of the system grows with the number of particles in the system. Also one could have expected that only the behavior on large time scales would matter since each interaction of the single particles clearly does matter on short time intervals but will not be relevant if one considers long time scales (the single interactions will effectively cancel each other and only an effective interaction potential, the mean field potential, will survive).

The standard procedure to derive a mean field equation for such a microscopic system is to consider

[2] This point is mostly ignored in the literature, e.g. in [6].

the reduced density matrices

$$\rho^{\psi_N}(x,y) = \int \psi_N(x, x_1, x_2, ..., x_N)\psi_N^*(y, x_1, x_2, ..., x_N)dx^2dx^3...dx^N \ .$$

This method is based on the fact that the time evolution of the reduced density matrices is given by the von Neumann equation

$$i\hbar\frac{\partial\rho}{\partial t} = [H, \rho]$$

where H is the Hamiltonian of the entire system. Hence, it is not sufficient to consider only the one-particle density matrix of the system since its time evolution depends on the reduced two-particle density matrices. Since the evolution of the reduced two-particle density matrices depends on the reduced density matrices for three particles and so forth, there exists a hierarchy of reduced density matrices. One main difficulty by deriving a mean field equation via this hierarchy of reduced density matrices is that it is necessary to regard all kinds of reduced density matrices and take the limit $N \to \infty$ which is a rather big effort since one has to take basically all types of interactions into consideration.

However, there is a much simpler (and even more powerful) procedure to derive mean field equations which is based on Grønwall's lemma (cf. 4.5). This method was invented by Pickl in [18] to derive the Hatree equation for a Bose gas. Using this method we will rigorously prove that the NSE is the correct mean field equation for a system described by (2.6).

For simplicity we shall begin with the derivation for identical bosons. This is also the case interesting for applications to some cosmological models, such as the inflation model (cf. e.g. [19]).

4.1 The Bosonic Case

In the following we consider a gas of identical bosons which is microscopically described by (4.1) resp. (4.2).

Definition 4.1. *Let* $\psi \in L^2(\mathbb{R}^{3N})$ *be a solution of* (4.1) *and* $\varphi(x_j) \in L^2(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$ *be a (bounded) solution of the Newton-Schrödinger equation* (1.2)

$$\begin{aligned} i\hbar\frac{\partial\varphi(x,t)}{\partial t} &= \left(-\frac{\hbar^2}{2m}\nabla^2 - Gm^2\int d^3x'\frac{|\varphi(x',t)|^2}{|x-x'|}\right)\varphi(x,t) \\ &= \left(-\frac{\hbar^2}{2m}\nabla^2 - |\varphi(x,t)|^2 * \frac{Gm^2}{x}\right)\varphi(x,t). \end{aligned} \tag{4.3}$$

Furthermore, assume that

$$\psi = \lim_{N\to\infty}\bigotimes_{j=1}^{N}\varphi_j. \tag{4.4}$$

Then we define $p_j^\varphi : L^2(\mathbb{R}^{3N}) \to L^2(\mathbb{R}^{3N})$

$$p_j^\varphi\psi(x_1, x_2, ..., x_N) = \varphi(x_j)\int \varphi^*(x_j)\psi(x_1, x_2, ..., x_N)d^3x_j \tag{4.5}$$

or shortly

$$p_j^\varphi = |\varphi(x_j)\rangle\langle\varphi(x_j)| \tag{4.6}$$

and $q_j^\varphi : L^2(\mathbb{R}^{3N}) \to L^2(\mathbb{R}^{3N})$

$$q_j^\varphi = 1 - p_j^\varphi \tag{4.7}$$

where 1 *denotes the identity.*

Lemma 4.2. *The operators* p_j^φ *and* q_j^φ *are projectors and thus have eigenvalues 0 and 1.*

Proof.

$$p_j^\varphi p_j^\varphi = |\varphi(x_j)\rangle \underbrace{\langle\varphi(x_j)|\varphi(x_j)\rangle}_{=1} \langle\varphi(x_j)| = p_j^\varphi \quad \Rightarrow \quad p_j^\varphi \text{ is a projector.}$$

This also implies that q_j^φ is a projector. As for all projectors the eigenvalues of p_j^φ, q_j^φ are 0 and 1 which follows from the fact that the eigenvalue equation for a projector can be written as

$$(p_j^\varphi)^2\psi = p_j^\varphi\psi \quad \Rightarrow \quad \lambda^2 - \lambda = 0 \quad \Rightarrow \quad \lambda \in \{0, 1\}.$$

□

Physically spoken, p_j^φ determines whether the j^{th} component of the wave function ψ resp. the j^{th} particle is the same as the wave function φ_j evolving due to the Newton-Schrödinger equation. q_j^φ has of course the opposite meaning.

The assumption (4.4) that the bosons are asymptotically in a product state, i.e. that they are nearly uncorrelated, is physically reasonable in many situations, e.g. in the cosmological inflation model (cf. [19]).

Now we compute the derivative of q_j^φ. This will be necessary to use Grønwall's lemma afterwards.

Lemma 4.3. *Let*

$$h = -\frac{\hbar^2}{2m}\nabla^2 - |\varphi(x,t)|^2 * \frac{Gm^2}{x} \tag{4.8}$$

be the Hamiltonian of the Newton-Schrödinger equation (4.3)*. Then the time derivative of* q_j^φ *is*

$$d_t q_j^\varphi = \frac{i}{\hbar}[h, p_j^\varphi] = -\frac{i}{\hbar}[h, q_j^\varphi] \tag{4.9}$$

where $[\cdot,\cdot]$ *denotes the commutator.*

Proof.

$$d_t q_j^\varphi \overset{(4.7)}{=} d_t\left(1 - p_j^\varphi\right) \overset{(4.6)}{=} -d_t|\varphi(x_j)\rangle\langle\varphi(x_j) \overset{(4.3)}{=} e^{-\frac{iht}{\hbar}} \underbrace{|\varphi(x_j)\rangle\langle\varphi(x_j)|}_{p_j^\varphi} e^{\frac{iht}{\hbar}} = \frac{i}{\hbar}[h, p_j^\varphi].$$

This last step is of course valid for arbitrary operators and nothing else than Heisenberg's equation of motion. □

Now, we are ready to introduce a quantity that counts the relative number of particles ψ not being described by the NSE (cf. [18]).

Definition 4.4. *Let $\langle\cdot\rangle_\psi = \langle\psi, \cdot\,\psi\rangle$ denote the expectation value of $\cdot$ w.r.t. ψ. Then we define*

$$\alpha_j^\varphi := \frac{1}{N}\sum_{j=1}^{N}\left\langle q_j^\varphi\right\rangle_\psi = \frac{1}{N}\sum_{j=1}^{N}\|q_j^\varphi\psi\|^2. \tag{4.10}$$

We remark that $0 \le \alpha^\varphi \le 1$ holds for any ψ and φ. We also note that

$$\alpha_j^\varphi = \alpha_i^\varphi \tag{4.11}$$

because of the symmetry of the wave function.

We shall prove in the following that under the condition that α_j^φ is small at one time, it remains small for all (physically relevant) times if the wave functions ψ and φ evolve according to the respective equations ((2.6) for ψ and the Newton-Schrödinger equation (4.3) for φ). Since the quantity α_j^φ gives the relative number of particles which are not in a product state of wave functions $\varphi(x_j)$, it is clear that if the value of $\alpha_j^\varphi(t)$ remains small for all times t it physically means that (4.3) describes effective behavior of the system very well and thus is the right mean field equation.

We shall estimate the time evolution of this quantity by aid of Grønwall's lemma[3].

Lemma 4.5 (Grønwall's lemma)**.** *Let $b^\varphi(t), c^\varphi(t) \in L^1([0,\infty)) \cap C^0([0,\infty))$ be continuous and integrable functions on $[0,\infty)$ with $c^\varphi(t) \ge 0$. If*

$$|d_t\alpha^\varphi(t)| \le b^\varphi(t)\alpha^\varphi(t) + c^\varphi(t) \tag{4.12}$$

the following holds:

$$\alpha^\varphi(t) \le \alpha^\varphi(0)exp\left(\int_0^t b^\varphi(\tau)d\tau\right) + \int_0^t c^\varphi(\tau)d\tau. \tag{4.13}$$

We don't give a proof of Grønwall's lemma since it is a standard lemma (for a proof see e.g. [20, 21]).

Grønwall's lemma is the key ingredient in the proof of the following theorem.

Theorem 4.6. *Let $\alpha^\varphi(t)$ be as in (4.10). Then*

$$\alpha^\varphi(t) \le exp\left(\int_0^t C_1^\varphi(\tau)d\tau\right)\alpha^\varphi(0) + C_2^\varphi\, t \tag{4.14}$$

[3] There are different versions of Grønwall's lemma. We state only that one which we will use afterwards (for an overview cf. [20]).

with $C_1^\varphi = \frac{GM^2}{\hbar\,[x]}\left(\frac{\sqrt{4\pi^2 D_j^{\varphi 2}+2\pi}}{2} + \sqrt{4\pi + \sqrt{2\pi} + 4\pi^2 D_j^{\varphi 2}}\right)$ *and* $C_2^\varphi = \frac{GM^2}{\hbar\,[x]} \frac{\sqrt{4\pi^2 D_j^{\varphi 2}+2\pi}}{2} \frac{1}{N}$ *where* $D_j^\varphi =$ $\operatorname{ess\,sup} \varphi(x_j)$ *and* $[x]$ *denotes the unit of length used in the respective (experimental) situation. In case of equidistant particles the constants* C_1^φ *and* C_2^φ *are independent of the particle.*

Proof. The independence of the constants C_1^φ and C_2^φ regarding the particle follows immediately from (4.11).

By virtue of Grønwall's lemma it suffices to show that

$$|d_t \alpha^\varphi(t)| \leq C_1^\varphi \alpha^\varphi(t) + C_2^\varphi. \tag{4.15}$$

Hence, we have to compute the derivative of $\alpha^\varphi(t)$.

Since all particles are identical bosons we can restrict ourselves on one particle, e.g. the j^{th} particle. Because of (4.11) we will sometimes drop the labels of α_j^φ and will write α for simplicity.

Let

$$H_j := -\frac{\hbar^2}{2m}\Delta_j - (N-1)^{-1} G m^2 \sum_{i \neq j} \frac{1}{|x_i - x_j|} \tag{4.16}$$

be the Hamiltonian of (4.1) for fixed j.

Using the Ehrenfest theorem we get

$$\begin{aligned} d_t \alpha^\varphi(t) &= d_t \left\langle q_j^\varphi \right\rangle_\psi = \frac{i}{\hbar}\left\langle [H_j, q_j^\varphi] \right\rangle_\psi + \left\langle (d_t q_j^\varphi) \right\rangle_\psi \overset{\text{lemma 4.3}}{=} \\ &= \frac{i}{\hbar}\left\langle [H_j, q_j^\varphi] \right\rangle_\psi - \frac{i}{\hbar}\left\langle [h_j, q_j^\varphi] \right\rangle_\psi = \frac{i}{\hbar}\left\langle [H_j - h_j, q_j^\varphi] \right\rangle_\psi. \end{aligned} \tag{4.17}$$

It should not be surprising that the difference $H_j - h_j$ between the Hamiltonian of the microscopic equation (4.1) and the one of the Newton-Schrödinger equation (4.3) shows up in the dynamics of α_j^φ since α is by definition the relative number of particles falsely described by the Newton-Schrödinger equation. We take a closer look on this difference.

$$\begin{aligned} H_j - h_j &= \left(-\frac{\hbar^2}{2m}\Delta_j - (N-1)^{-1} G m^2 \sum_{i \neq j} \frac{1}{|x_i - x_j|}\right) - \left(-\frac{\hbar^2}{2m}\Delta_j - |\varphi_j(x,t)|^2 * \frac{Gm^2}{x}\right) = \\ &= |\varphi_j(x,t)|^2 * \frac{Gm^2}{x_j} - (N-1)^{-1} G m^2 \sum_{i \neq j} \frac{1}{|x_i - x_j|} \overset{\substack{\text{identical} \\ \text{bosons}}}{=} \underbrace{|\varphi_j(x,t)|^2 * \frac{Gm^2}{x_j} - Gm^2 \frac{1}{|x_i - x_j|}}_{:= U_{ij}} \end{aligned}$$

where we also fixed i w.l.o.g. and therefore drop the factor $N-1$. The only term that does not cancel out in this difference is the difference of the potentials which we call U_{ij} from now on. Substituting this in (4.17) yields

$$d_t \alpha_j^\varphi(t) = \frac{i}{\hbar}\left\langle [U_{ij}, q_j^\varphi] \right\rangle_\psi = \frac{i}{\hbar}\left(\left\langle U_{ij} q_j^\varphi \right\rangle_\psi - \left\langle q_j^\varphi U_{ij} \right\rangle_\psi\right) =$$

$$= \frac{i}{\hbar}\left(\left\langle \underbrace{(p_j^\varphi + q_j^\varphi)}_{=1} \underbrace{(p_i^\varphi + q_i^\varphi)}_{=1} U_{ij} q_j^\varphi \underbrace{(p_i^\varphi + q_i^\varphi)}_{=1} \right\rangle_\psi - \left\langle \underbrace{(p_i^\varphi + q_i^\varphi)}_{=1} q_j^\varphi U_{ij} \underbrace{(p_j^\varphi + q_j^\varphi)}_{=1} \underbrace{(p_i^\varphi + q_i^\varphi)}_{=1} \right\rangle_\psi \right) =$$
$$= \frac{i}{\hbar}(\left\langle p_j^\varphi p_i^\varphi U_{ij} q_j^\varphi p_i^\varphi \right\rangle_\psi + \left\langle p_j^\varphi q_i^\varphi U_{ij} q_j^\varphi p_i^\varphi \right\rangle_\psi + \left\langle q_j^\varphi p_i^\varphi U_{ij} q_j^\varphi p_i^\varphi \right\rangle_\psi + \left\langle q_j^\varphi q_i^\varphi U_{ij} q_j^\varphi p_i^\varphi \right\rangle_\psi +$$
$$+ \left\langle p_j^\varphi p_i^\varphi U_{ij} q_j^\varphi q_i^\varphi \right\rangle_\psi + \left\langle p_j^\varphi q_i^\varphi U_{ij} q_j^\varphi q_i^\varphi \right\rangle_\psi + \left\langle q_j^\varphi q_i^\varphi U_{ij} q_j^\varphi q_i^\varphi \right\rangle_\psi -$$
$$- \left\langle q_j^\varphi p_i^\varphi U_{ij} p_j^\varphi p_i^\varphi \right\rangle_\psi - \left\langle q_j^\varphi q_i^\varphi U_{ij} p_j^\varphi p_i^\varphi \right\rangle_\psi - \left\langle q_j^\varphi p_i^\varphi U_{ij} q_j^\varphi p_i^\varphi \right\rangle_\psi - \left\langle q_j^\varphi q_i^\varphi U_{ij} q_j^\varphi p_i^\varphi \right\rangle_\psi -$$
$$- \left\langle q_j^\varphi p_i^\varphi U_{ij} p_j^\varphi q_j^\varphi \right\rangle_\psi - \left\langle q_j^\varphi p_i^\varphi U_{ij} q_j^\varphi q_i^\varphi \right\rangle_\psi - \left\langle q_j^\varphi q_i^\varphi U_{ij} q_j^\varphi q_i^\varphi \right\rangle_\psi) =$$
$$= \frac{i}{\hbar}(\left\langle p_j^\varphi q_i^\varphi U_{ij} q_j^\varphi p_i^\varphi \right\rangle_\psi + \left\langle p_j^\varphi p_i^\varphi U_{ij} q_j^\varphi p_i^\varphi \right\rangle_\psi + \left\langle p_j^\varphi p_i^\varphi U_{ij} q_j^\varphi q_i^\varphi \right\rangle_\psi + \left\langle p_j^\varphi q_i^\varphi U_{ij} q_j^\varphi q_j^\varphi \right\rangle_\psi -$$
$$- \left\langle q_j^\varphi p_i^\varphi U_{ij} p_j^\varphi q_i^\varphi \right\rangle_\psi - \left\langle q_j^\varphi p_i^\varphi U_{ij} p_j^\varphi p_i^\varphi \right\rangle_\psi - \left\langle q_j^\varphi q_i^\varphi U_{ij} p_j^\varphi p_i^\varphi \right\rangle_\psi - \left\langle q_j^\varphi q_i^\varphi U_{ij} p_j^\varphi q_i^\varphi \right\rangle_\psi) \tag{4.18}$$

We now analyze the different terms to get a upper bound for $d_t \alpha_j^\varphi(t)$.

$$\left\langle p_j^\varphi q_i^\varphi U_{ij} q_j^\varphi p_i^\varphi \right\rangle_\psi - \left\langle q_j^\varphi p_i^\varphi U_{ij} p_j^\varphi q_i^\varphi \right\rangle_\psi \overset{\text{"exchange" } i \text{ and } j}{=\!=} 0 \tag{4.19}$$

Since ψ is symmetric under exchange of particles, one can rename in the second term the i$^{\text{th}}$ and j$^{\text{th}}$ particles to cancel the first term.

For estimating the other terms of (4.18) it is helpful to note that each summand appears together with its complex conjugated. This follows immediately from the definition of q_j^φ (cf. definition 4.1). Thus, since we are looking for a upper bound for the absolute value of (4.18) we can neglect the complex conjugated summands. Therefore (4.18) reduces by taking the absolute value to

$$|d_t \alpha_j^\varphi(t)| = \frac{1}{\hbar}\left(\left\langle p_j^\varphi p_i^\varphi U_{ij} q_j^\varphi p_i^\varphi \right\rangle_\psi + \left\langle p_j^\varphi p_i^\varphi U_{ij} q_j^\varphi q_i^\varphi \right\rangle_\psi + \left\langle p_j^\varphi q_i^\varphi U_{ij} q_j^\varphi q_j^\varphi \right\rangle_\psi \right) \tag{4.20}$$

Hence there are only three terms left.

Next, we want to estimate the term

$$\left\langle p_j^\varphi p_i^\varphi U_{ij} q_j^\varphi p_i^\varphi \right\rangle_\psi. \tag{4.21}$$

Therefore we first focus ourselves on $p_i^\varphi U_{ij} p_i^\varphi$ since this will be the important part.

$$p_i^\varphi U_{ij} p_i^\varphi = |\varphi(x_i)\rangle\langle\varphi(x_i)|\left(|\varphi(x_j)|^2 * \frac{Gm^2}{x_j} - Gm^2 \frac{1}{|x_i - x_j|}\right)|\varphi(x_i)\rangle\langle\varphi(x_i) =$$
$$= |\varphi(x_i)\rangle\langle\varphi(x_i)|\; |\varphi(x_j)|^2 * \frac{Gm^2}{x_j}|\varphi(x_i)\rangle\langle\varphi(x_i) -$$
$$- Gm^2|\varphi(x_i)\rangle \underbrace{\langle\varphi(x_i)|\frac{1}{|x_i - x_j|}|\varphi(x_i)\rangle}_{\substack{=\int \frac{1}{|x_i - x_j|}|\varphi(x_i)|^2 dx_i \\ = \frac{1}{x_j} * |\varphi(x_j)|^2}} \langle\varphi(x_i) \overset{p_i^\varphi p_i^\varphi = p_i^\varphi}{=} 0 \tag{4.22}$$

where we used that the discrete convolution in the last line becomes a usual convolution by taking the limit $N \to \infty$.

From this computation it is clear that (4.21) vanishes since q_j and p_i commute. For this term to vanish it was essential that we had scaled (4.1) in the right way. We remark also that only the NSE yields the term vanishing. This fact can be regarded as a first hint that the NSE is the right effective equation for the microscopic system described by (2.6) resp. (4.1).

The next term of (4.18) we want to estimate is

$$\left\langle p_j^\varphi p_i^\varphi U_{ij} q_j^\varphi q_i^\varphi \right\rangle_\psi . \tag{4.23}$$

Splitting U_{ij} yields

$$\begin{aligned}\left\langle p_j^\varphi p_i^\varphi U_{ij} q_j^\varphi q_i^\varphi \right\rangle_\psi &= Gm^2 \left(\left\langle p_j^\varphi p_i^\varphi \left(\varphi(x_j) * \frac{1}{x_j} \right) q_j^\varphi q_i^\varphi \right\rangle_\psi - \left\langle p_j^\varphi p_i^\varphi \frac{1}{|x_i - x_j|} q_j^\varphi q_i^\varphi \right\rangle_\psi \right) \overset{p_i^\varphi q_i^\varphi = 0}{=} \\ &= -Gm^2 \left\langle p_j^\varphi p_i^\varphi \frac{1}{|x_i - x_j|} q_j^\varphi q_i^\varphi \right\rangle_\psi .\end{aligned} \tag{4.24}$$

In the last step we have used that the potential of the Newton-Schrödinger equation depends "only on the j^{th} particle"[4] and we therefore can pull the q_i^φ to the p_i^φ through it. This yields the term with the Newton-Schrödinger potential vanish since these two projectors are orthogonal to each other.

Next, we sum all possible i and drop the factor $N-1$ and this leads by the Cauchy-Schwarz inequality (CS) to:

$$\begin{aligned}Gm^2 \left\langle p_j^\varphi p_i^\varphi \frac{1}{|x_i - x_j|} q_j^\varphi q_i^\varphi \right\rangle_\psi &= Gm^2 \frac{1}{N-1} \left\langle \psi, \underbrace{\sum_{i \neq j} p_j^\varphi p_i^\varphi \frac{1}{|x_i - x_j|} q_i^\varphi}_{:=\omega} q_j^\varphi \psi \right\rangle \overset{\text{CS}}{\leq} \\ &\leq Gm^2 \frac{1}{N-1} \|\omega \psi\| \|q_j^\varphi \psi\| \overset{(4.10)}{=} Gm^2 \|\omega\psi\|_2 \, |\sqrt{\alpha}|\end{aligned} \tag{4.25}$$

Computing the norm squared of $\omega\psi$ yields

$$\begin{aligned}\|\omega\psi\|_2^2 &= \left\langle \sum_{i \neq j \neq k} p_j^\varphi p_i^\varphi \frac{1}{|x_i - x_j|} q_i^\varphi q_k^\varphi \frac{1}{|x_k - x_j|} p_j^\varphi p_k^\varphi \right\rangle_\psi = \\ &= \left\langle \sum_{i \neq j} p_j^\varphi p_i^\varphi \frac{1}{|x_i - x_j|} q_i^\varphi \frac{1}{|x_i - x_j|} p_j^\varphi p_i^\varphi \right\rangle_\psi + \left\langle \sum_{\substack{i \neq j \neq k \\ i \neq k}} p_j^\varphi p_i^\varphi \frac{1}{|x_i - x_j|} q_i^\varphi q_k^\varphi \frac{1}{|x_k - x_j|} p_j^\varphi p_k^\varphi \right\rangle_\psi = \\ &= \left\langle \sum_{i \neq j} p_j^\varphi p_i^\varphi \frac{1}{|x_i - x_j|} q_i^\varphi \frac{1}{|x_i - x_j|} p_j^\varphi p_i^\varphi \right\rangle_\psi + \left\langle \sum_{\substack{i \neq j \neq k \\ k \neq i}} q_k^\varphi p_j^\varphi p_i^\varphi \frac{1}{|x_i - x_j|} \frac{1}{|x_k - x_j|} p_j^\varphi p_k^\varphi q_i^\varphi \right\rangle_\psi \underset{\text{CS}}{\overset{\|q_i^\varphi\|_{\text{op}} \leq 1}{\leq}}\end{aligned}$$

[4]Of course, the potential depends implicitly on all particles via the convolution (cf. the discussion following in section 5) but it is formally evaluated on the j^{th} particle.

$$\leq \left\langle \sum_{i\neq j} p_i^\varphi p_j^\varphi \frac{1}{|x_i-x_j|^2} p_j^\varphi p_i^\varphi \right\rangle_\psi + \underbrace{\|q_k^\varphi \psi\|}_{=\sqrt{\alpha}} \left\langle \sum_{\substack{i\neq j\neq k\\ k\neq i}} p_i^\varphi p_j^\varphi \frac{1}{|x_i-x_j|} \frac{1}{|x_k-x_j|} p_j^\varphi p_k^\varphi \right\rangle_\psi \underbrace{\|q_i^\varphi \psi\|}_{=\sqrt{\alpha}} \overset{\|p_m^\varphi\|_{\text{op}}\leq 1}{\underset{\text{CS}}{\leq}}$$

$$\leq (N-1) \underbrace{\left\| p_j^\varphi \frac{1}{|x_i-x_j|^2} p_j^\varphi \right\|_{\text{op}}}_{:=I} + \alpha(N^2-N-1) \underbrace{\left\| p_j^\varphi \frac{1}{|x_i-x_j|} \frac{1}{|x_k-x_j|} p_j^\varphi \right\|_{\text{op}}}_{:=K} \tag{4.26}$$

where we have used that the operator norm of an arbitrary projector is less than or equal to 1. Next, we would like to bound I and K from the top.

The difficulty thereby is however that $\frac{1}{x}$ is not in $L^p(\mathbb{R}^3)$ for any p. But it belongs to $L^p(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)\ \forall p < 3$, i.e. the following holds:

$$\forall\ 0 < \delta < \infty : \left(\frac{1}{r} \in L^p(\mathbb{R}^3)\ \forall r \leq \delta\right) \wedge \left(\frac{1}{r} \in L^\infty(\mathbb{R}^3)\ \forall r > \delta\right). \tag{4.27}$$

Hence one can split the potential into two parts

$$f_\delta := \begin{cases} \frac{1}{|x_i-x_j|} & \forall\ |x_i-x_j| \leq \delta \\ 0 & \text{else} \end{cases} \quad \text{and} \quad g_\delta := \begin{cases} \frac{1}{|x_i-x_j|} & \forall\ |x_i-x_j| > \delta \\ 0 & \text{else} \end{cases} \tag{4.28}$$

Clearly $f_\delta \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$ and $g_\delta \in L^\infty(\mathbb{R}^3)$ as well as $f_\delta + g_\delta = |x_i - x_j|^{-1}$ holds.

In order to determine the optimal value of δ we shortly regard δ as a dimensionless parameter and will restore the unit afterwards. We note that $\|g_\delta\|_\infty = \frac{1}{\delta}$. Moreover $\|f_\delta\|_1 = 4\pi \int_0^\delta r dr = 2\pi\delta^2$ holds.[5] By putting these expressions for the norms $\|f_\delta\|_1$ and $\|g_\delta\|_\infty$ equal we get an optimal value of δ

$$\delta_{\text{opt}} = (2\pi)^{-\frac{1}{4}}. \tag{4.29}$$

This is thus the value at which we cut the potential. Plugging δ_{opt} into $\|f_\delta\|_1$ and $\|g_\delta\|_\infty$ and restoring the units yields

$$\|f\|_1 := \|f_{\delta_{\text{opt}}}\|_1 = \sqrt{2\pi}\big[x^{-1}\big] \quad \|g\|_\infty := \|g_{\delta_{\text{opt}}}\|_\infty = (2\pi)^{\frac{1}{4}}\big[x^{-1}\big] \tag{4.30}$$

where the squared bracket $[x^{-1}]$ denotes the unit of x^{-1}, i.e. the inverse of the unit in which distances and coordinates are measured.

Furthermore, we will use the assumption that $\varphi(x_j) \in L^\infty(\mathbb{R}^3)$ (cf. 4.1), i.e.

$$\operatorname*{ess\,sup}_{x_j} \varphi(x_j) =: D_j^\varphi < \infty. \tag{4.31}$$

[5]For the computation of $\|f_\delta\|_1$ we used that $\|\frac{1}{r}\|_p = \left(4\pi \int_0^\infty s^{2-p} ds\right)^{\frac{1}{p}}\ \forall\ r \in \mathbb{R}^3)$ (cf. [22]).

Plugging all that into I and using the triangle inequality as well as Hölder's inequality (HI) yields

$$
\begin{aligned}
I &= \left\| |\varphi(x_j)\rangle\langle\varphi(x_j)| \frac{1}{|x_i - x_j|^2} |\varphi(x_j)\rangle\langle\varphi(x_j)| \right\|_{\mathrm{op}} \leq \\
&\leq |\varphi(x_j)\rangle \big(\langle\varphi(x_j)| f^2 |\varphi(x_j)\rangle + \langle\varphi(x_j)| g^2 |\varphi(x_j)\rangle \big) \langle\varphi(x_j)| \overset{\mathrm{HI}}{\leq} \\
&\leq |\varphi(x_j)\rangle \left(\underbrace{\|f\|_1^2}_{=4\pi^2[x^{-1}]^2} \underbrace{\|\varphi(x_j)\|_\infty^2}_{\leq D_j^{\varphi 2}} + \underbrace{\|g\|_\infty^2}_{=2\pi[x^{-1}]^2} \underbrace{\|\varphi(x_j)\|_1^2}_{=1} \right) \langle\varphi(x_j)| \leq \left(4\pi^2 D_j^{\varphi 2} + 2\pi\right)\left[x^{-1}\right]^2. \qquad (4.32)
\end{aligned}
$$

The same bound holds for K since we can use the same partition of the potential for both the i$^{\text{th}}$ and the k$^{\text{th}}$ particle due to the symmetry of the wave function under exchange of particles.

$$
\begin{aligned}
K &= \left\| |\varphi(x_j)\rangle\langle\varphi(x_j)| \frac{1}{|x_i - x_j|} \frac{1}{|x_k - x_j|} |\varphi(x_j)\rangle\langle\varphi(x_j)| \right\|_{\mathrm{op}} \leq \\
&\leq |\varphi(x_j)\rangle \big(\langle\varphi(x_j)| f^2 |\varphi(x_j)\rangle + \langle\varphi(x_j)| g^2 |\varphi(x_j)\rangle \big) \langle\varphi(x_j)| \overset{\mathrm{HI}}{\leq} \\
&\leq \cdots \leq \left(4\pi^2 D_j^{\varphi 2} + 2\pi\right)\left[x^{-1}\right]^2 \qquad (4.33)
\end{aligned}
$$

Returning to (4.26) this leads to

$$
\begin{aligned}
\|\omega\psi\|_2^2 &\leq (N-1)\left(2\pi D_j^{\varphi 2} + \sqrt{2\pi}\right)\left[x^{-1}\right]^2 + \alpha(N^2 - N - 1)\left(2\pi D_j^{\varphi 2} + \sqrt{2\pi}\right)\left[x^{-1}\right]^2 \leq \\
&\leq \left((N^2 - 1)(\alpha + \underbrace{\frac{N-1}{N^2-1}}_{=\frac{1}{N+1}} \right) \left(4\pi^2 D_j^{\varphi 2} + 2\pi\right)\left[x^{-1}\right]^2. \qquad (4.34)
\end{aligned}
$$

Plugging this bound into (4.25) yields an upper bound for the absolute value of (4.23)

$$
\begin{aligned}
|\left\langle p_j^\varphi p_i^\varphi U_{ij} q_j^\varphi q_i^\varphi \right\rangle_\psi| &\overset{(4.24)}{=} Gm^2 \left\langle p_j^\varphi p_i^\varphi \frac{1}{|x_i - x_j|} q_j^\varphi q_i^\varphi \right\rangle_\psi \overset{(4.25)}{\leq} Gm^2 \frac{1}{N-1} \|\omega\psi\|_2 \sqrt{\alpha} \overset{(4.34)}{\leq} \\
&\leq Gm^2\left[x^{-1}\right] \frac{1}{N-1} \sqrt{\alpha \left((N^2-1)\left(\alpha + \frac{1}{N+1}\right)\right) \left(4\pi^2 D_j^{\varphi 2} + 2\pi\right)} \underset{\mathrm{AGM}}{\overset{\mathrm{conv}}{\leq}} \\
&\leq Gm^2\left[x^{-1}\right] \frac{1}{2} \frac{1}{N-1} (N-1) \sqrt{4\pi^2 D_j^{\varphi 2} + 2\pi} \left(\alpha + \frac{1}{N+1}\right) \leq \\
&\leq Gm^2\left[x^{-1}\right] \frac{\sqrt{4\pi^2 D_j^{\varphi 2} + 2\pi}}{2} \left(\alpha + \frac{1}{N}\right). \qquad (4.35)
\end{aligned}
$$

We used in the step between the second and the third row the convexity of the square root (conv) $\sqrt{a+b} \leq \sqrt{a} + \sqrt{b}$ as well as the arithmetic-geometric mean inequality (AGM) $\sqrt{ab} \leq \frac{a+b}{2}$ (both valid for any $a, b > 0$).

The last summand of (4.20) we have to bound is

$$\left\langle p_j^\varphi q_i^\varphi U_{ij} q_j^\varphi q_i^\varphi \right\rangle_\psi .$$

By the Cauchy-Schwarz inequality we determine

$$\left\langle p_j^\varphi q_i^\varphi U_{ij} q_j^\varphi q_i^\varphi \right\rangle_\psi \overset{\text{CS}}{\leq} \underbrace{\|q_i^\varphi \psi\|_2}_{=\sqrt{\alpha_i^\varphi}} \|p_j^\varphi U_{ij}\|_{\text{op}} \underbrace{\|q_j^\varphi\|_{\text{op}}}_{\leq 1} \underbrace{\|q_i^\varphi \psi\|_2}_{=\sqrt{\alpha_i^\varphi}} \leq \|p_j^\varphi U_{ij}\|_{\text{op}} \alpha_i^\varphi \tag{4.36}$$

Computing $\|p_j^\varphi U_{ij}\|_{\text{op}}^2$ yields

$$\begin{aligned} \|p_j^\varphi U_{ij}\|_{\text{op}}^2 &= G^2 m^4 \|p_j^\varphi \left(\frac{1}{x_j} * |\varphi(x_j)|^2 - \frac{1}{|x_i - x_j|}\right)^2 p_j^\varphi\|_{\text{op}} \leq \\ &\leq G^2 m^4 (|\varphi(x_j)\rangle \underbrace{\langle \varphi(x_j) \left(|\frac{1}{x_j} * |\varphi(x_j)|^2 \right)^2 |\varphi(x_j)\rangle}_{:=L} \langle \varphi(x_j)| + \\ &+ |\varphi(x_j)\rangle \underbrace{\langle \varphi(x_j)| \frac{1}{|x_i - x_j|^2} |\varphi(x_j)\rangle}_{\overset{(4.32)}{\leq} 4\pi^2 D_j^{\varphi 2} + 2\pi} \langle \varphi(x_j)|)\left[x^{-1}\right]^2 \end{aligned} \tag{4.37}$$

where we recognize that the second summand is exactly the same as I which we already have estimated in (4.32).

We now have to find a bound for the convolution term L. The distributivity of the convolution allows us to split the convolution recalling that $f_\delta + g_\delta = \frac{1}{|x_i - x_j|}$ (cf. (4.28)). We can then use Young's inequality (YI) $\|a * b\|_p \leq \|a\|_q \|b\|_r$ where $\frac{1}{q} + \frac{1}{r} = 1 + \frac{1}{p}$.

$$\begin{aligned} L &= \langle \varphi(x_j)| \left((f_\delta + g_\delta) * |\varphi|^2\right)^2 |\varphi(x_j)\rangle \leq \\ &\leq \langle \varphi| \left(f_\delta * |\varphi(x_j)|^2\right)^2 \varphi(x_j)\rangle + \langle \varphi(x_j)| \left(g_\delta * |\varphi(x_j)|^2\right)^2 |\varphi(x_j)\rangle \overset{\text{YI}}{\leq} \\ &\leq \underbrace{\|f\|_1^2}_{2\pi[x^{-1}]^2} \underbrace{\|\varphi(x_j)\|_1^2}_{=1} + \underbrace{\|g\|_\infty^2}_{\sqrt{2\pi}[x^{-1}]^2} \underbrace{\|\varphi(x_j)\|_1^2}_{=1} = \left(2\pi + \sqrt{2\pi}\right)\left[x^{-1}\right]^2 \end{aligned} \tag{4.38}$$

For the first convolution we have chosen the coefficients for Young's inequality as $p = q = r = 1$ (since $f \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$), whereas for the second $p = q = \infty, r = 1$ (since $g \in L^\infty(\mathbb{R}^3)$).

Plugging the bound of L into (4.37) yields for (4.36)

$$\left\langle p_j^\varphi q_i^\varphi U_{ij} q_j^\varphi q_i^\varphi \right\rangle_\psi \overset{(4.36)}{\leq} \|p_j^\varphi U_{ij}\|_{\text{op}} \alpha \overset{(4.37)}{\leq} G m^2 \left[x^{-1}\right] \sqrt{4\pi + \sqrt{2\pi} + 4\pi^2 D_j^{\varphi 2}}\, \alpha \tag{4.39}$$

Now, we have estimated all summands appearing in (4.20).

Thus, we get as upper bound for $|d_t \alpha_j^\varphi|$ in total

$$\begin{aligned}
|d_t \alpha_j^\varphi| &\overset{(4.20)}{\leq} \frac{1}{\hbar} \left(\underbrace{\left\langle p_j^\varphi p_i^\varphi U_{ij} q_j^\varphi p_i^\varphi \right\rangle_\psi}_{=0} + \underbrace{\left\langle p_j^\varphi p_i^\varphi U_{ij} q_j^\varphi q_i^\varphi \right\rangle_\psi}_{\overset{(4.35)}{\leq} Gm^2[x^{-1}] \frac{\sqrt{4\pi^2 D_j^{\varphi 2} + 2\pi}}{2} (\alpha + \frac{1}{N})} + \underbrace{\left\langle p_j^\varphi q_i^\varphi U_{ij} q_j^\varphi q_j^\varphi \right\rangle_\psi}_{\overset{(4.39)}{\leq} Gm^2[x^{-1}] \sqrt{4\pi + \sqrt{2\pi} + 4\pi^2 D_j^{\varphi 2}}\, \alpha} \right) \leq \\
&\leq \frac{1}{\hbar} Gm^2 [x^{-1}] \left(\frac{\sqrt{4\pi^2 D_j^{\varphi 2} + 2\pi}}{2} + \sqrt{4\pi + \sqrt{2\pi} + 4\pi^2 D_j^{\varphi 2}} \right) \alpha_j^\varphi + \frac{1}{\hbar} Gm^2 [x^{-1}] \frac{\sqrt{4\pi^2 D_j^{\varphi 2} + 2\pi}}{2} \frac{1}{N} = \\
&= C_1^\varphi \alpha + C_2^\varphi
\end{aligned} \tag{4.40}$$

Applying Grønwall's lemma completes the proof of the theorem.

□

We recap the physical meaning of the theorem briefly. Given a initial value $\alpha(0)$ of the relative number of particles that are not in a product state at time $t = 0$. Then the theorem provides an upper bound for the relative number of particles not being in the state which is a product state at any time t of wave functions evolved due to the NSE.

Since $N \to \infty$ the second summand of the upper bound $C_2^\varphi t$ becomes arbitrarily small. Because of the assumption that the bosons initially are almost in a product state $\alpha(0)$ is very closed to 0 and for times small enough the first summand also is very small despite the exponential increase with time.

To see why the physically relevant times are small enough we remind that we scaled the time of the Newton-Schrödinger equation by a factor $(N-1)^{-2}$ in order to compensate the additional summands in the double sum in the potential energy compared with the kinetic energy (see the discussion before (4.2)). That means however that the time scale we regarded in the theorem is $(N-1)^2$ times larger than the real physical time scale. Hence, since $N \to \infty$, all physically relevant time scales are very short when scaling them like in the theorem.

The theorem states that if the particle number N is very large and α is small at one particular time α stays small for all (physically relevant) times. The time evolution of α can be interpreted as the difference between the real evolution of the system and the one described by the mean field since α is the relative number of particles which are not in the product state described by the product of the mean field wave functions. Hence, the mean field behavior of the a system consisting of identical bosons evolving due to (2.6) is described by the Newton-Schrödinger equation.

Moreover, the theorem provides estimates for the errors coming from the facts that one does never have an infinite number of particles in reality, and that the assumption that $\alpha(0) = 0$ does not hold in any experimental setting. By the theorem one can estimate these errors when knowing the particle number N, the supremum D_j^φ of φ and the value of α at one particular time.

We emphasize that the wave function φ appearing in the Newton-Schrödinger equation does not describe the evolution of any particle but only the evolution of the effective mean field of all the particles. It is a collective variable of the whole system (cf. also [7]). This collective variable is sometimes also called the center of mass (cf. e.g. [23]). In section 5 we provide a more detailed discussion on that issue.

4.2 Possible Generalizations

We want to mention some possible generalizations of the proof we provided in sec. 4 for identical bosons.

First, we note that the scheme of the proof can be generalized to a mixture of two different kinds of bosons with only a little more mathematical effort. This has been done in [21] for potentials that are in some L^p space. As explained before, the potential of the Newton-Schrödinger equation does not be in any L^p space but can be split into two parts being in different L^p spaces (cf. (4.28). Hence, combining our proof and [21] yields that the Newton-Schrödinger equation is valid as mean field equation for a mixture of two types of bosons. Undoubtedly one can generalize this result to an arbitrary number of types of bosons. One key ingredient in [21] is, however, that the bosons do not change their types during the evolution. Without that assumption, the proof would be much more complicated and we are not aware of any rigorous results in this direction.

Another point is that our proof can be generalized to systems with a large volume but a small density (cf. [24]). Also there the only difference to the proof in [24] is the splitting of the potential (4.28).

So far we considered only bosonic systems. However, there are also results which indicate that the Newton-Schrödinger equation can be derived from (2.6) as a mean field equation also for fermions. However, mean field equations for fermionic systems are content of current research.

Deriving them is much more complicated than for bosons. This is due to the fact that according to Pauli's exclusion principle each fermion has to be separated from the others, i.e. the size of the system scales differently with the number of particles than for bosons. Furthermore, in our proof we used the symmetry of the wave function several times which makes the generalization to fermionic systems rather difficult.

Nevertheless, there have been made a lot of progress in proofing the mean field behavior of fermionic systems in recent years.

One approach is to consider states which can in leading order be described as classical systems.[6] This ansatz is taken in [25, 26]. Since they use a rather different method of proving the mean field equation than the one we used in our proof for bosons, we do not go into the details. However, it should be clear that it only can applied to special systems.

There are, however, also results which are based on the method of our derivation in sec. 4. In [27, 28] the mean field limit of a fermionic system is derived under certain conditions. One of these is that the initial wave function of the system is approximately a Slater determinant which is the analogous

[6]These states are called "semiclassical" in the literature. However, this has nothing to do with semiclassical gravity but simply refers to the fact that the states can be approximately described by the classical Vlasov equation.

assumption to being in a product state (cf. eq. (4.4)) for fermionic systems. Especially the methods of [28] can be applied to the problem of proving that the Newton-Schrödinger equation describes the mean field evolution of a system of fermions which wave functions are described by (2.6). Therefore, one has to bound the initial kinetic energy of the system and furthermore restrict its scaling behavior.

Relaxing these constraints is a topic of current research.

5 Role of the Newton-Schrödinger Equation in the Literature

The Newton-Schrödinger equation appears in the literature in very different contexts. We now give an critical overview of the most common ones.

Historically, the Newton-Schrödinger equation was introduced first by Diòsi [29] and Penrose [30–32] in order to explain the collapse of the wave function. At first glance, this seems to make sense since a wave function ψ evolving due to the Newton-Schrödinger equation does concentrates itself because of the attractive gravitational potential. But as explained below that does not yield Born's law.

The Newton-Schrödinger equation is very often interpreted as a equation describing the evolution of one single particle. Therefore, it is derived from semiclassical gravity but in a slightly different way we have done it (cf. [6, 29]). For this derivation one has to assume that semiclassical gravity is fundamental, i.e. that the gravitational field is classically even at a fundamental level. However, this assumption has been criticized by many physicists for both philosophical and physical reasons (cf. e.g. [7, 33, 34]). However, in the view of some physicists the arguments are not yet excluding the possibility for semiclassical gravity being the fundamental theory (cf. e.g. [6]) and they are looking for some experimental result that decides that question whether there is a underlying quantum theory of semiclassical gravity or not (cf. e.g. [35]). We will not go into this discussion deeply here (for a rather comprehensive overview of the arguments for and against a fundamental treatment of semiclassical gravity see [8] and the references therein).

However, in our view it is rather clear that semiclassical gravity cannot be a fundamental theory. One main reason for this is that taking the expectation value of some quantity like it is done in the semiclassical Einstein equations (2.2) is only meaningful if one regards more than one particle/field since it is a stochastic computation. Furthermore, the expectation value is taken with respect to a state of a quantum field. Since the states of quantum fields can generally attributed to different particle numbers, the number of particles with respect to which the expectation value is taken is not fixed (cf. e.g. [5]). And if one agrees on that, semiclassical gravity is already an effective theory that describes a mean field motion of a many particle system.

Another aspect is that the expectation value of the energy-momentum-tensor is generally not covariantly conserved while the Einstein tensor of classical general relativity is, i.e. $\nabla_\mu \langle T^{\mu\nu}\rangle_\phi \neq 0 = \nabla_\mu G^{\mu\nu}$ (cf. e.g. [36]). That means that the semiclassical Einstein equations can only be valid in a certain regime.

Moreover, in [36, 37] Page and Geiger developed a thought experiment which proves that semiclassical gravity cannot be a fundamental theory, at least for the Many-Worlds interpretation of quantum physics. The situation they consider is that of two separated massive macroscopic objects, e.g. stars.

According to semiclassical gravity there is no difference between this situation and one of only one object in the center of the two. This is due to the manner how the expectation value changes when regarding a superposition (see also e.g. [6, 38].

If one regards the Newton-Schrödinger equation as a equation describing one single particle one has to regard semiclassical gravity as fundamental and derive the Newton-Schrödinger equation from it (cf. e.g. [6, 23]). However, this is in conflict to the reasoning given before that semiclassical gravity is already an effective theory for many particles. Hence, the Newton-Schrödinger equation cannot be an equation describing the motion of one single particle despite the fact that it looks like such a single particle equation at first glance.

Nevertheless, it is important to note that the Newton-Schrödinger equation gives rise to a continuity equation for $|\psi|^2$

$$\frac{\partial}{\partial t}|\psi(x,t)|^2 = \nabla \cdot \left(\frac{i\hbar}{m}\mathrm{Im}\big(\psi^* \nabla \psi\big)\right). \tag{5.1}$$

where Im denotes the imaginary part. This follows from the fact that the potential (i.e. the convolution term) in the Newton-Schrödinger equation is real. Hence, an interpretation of $|\psi|$ as probability amplitude seems to be reasonable. At first glance, this is also valid for an interpretation of the Newton-Schrödinger equation as one particle equation.

But this does not mean that the Newton-Schrödinger equation is consistent with Born's law (cf. e.g. [6, 39]). To see this we write the wave function in the polar form $\psi = Re^{iS}$ with $R, S \in \mathbb{R}$. Plugging this form into the Newton-Schrödinger equation ß, (1.2) yields

$$i\frac{\partial R}{\partial t} - R\frac{\partial S}{\partial t} = -\frac{\hbar}{2m}\big(\Delta R + 2i\nabla R \nabla S + -R(\nabla S)^2 + iR\Delta S\big) - Gm^2R^3. \tag{5.2}$$

The real part of this equation depends[7] cubicly on the amplitude R of the wave function. Hence, the wave function changes its shape during the evolution in a very non-linear manner. This non-linearity implies that the wave function focus itself. This, of course, can been seen also directly from the original Newton-Schrödinger equation (1.2). That process of self-focusing gives rise to several conceptual problems. For example, it seems to allow superluminal signaling (cf. [6] for details and other problems). Moreover, the Newton-Schrödinger equation cannot explain the collapse of the wave function since (similarly to semiclassical gravity) the Newton-Schrödinger equation cannot be applied to macroscopic superpositions. If so, the results are not physically reasonable. In the example of two macroscopicly disjoint states, the resulting wave function would again be such that it "collapses" right in the middle of the two states. This is a contradiction to Born's law (cf. [6, 39]).

There are proposals of extensions of the Newton-Schrödinger equation in realistic formulations of quantum physics which do not seem to have these kinds of problems (see [39] for a proposal in context of the GRWm-theory[8] and [38] for one in context of Bohmian mechanics). However, it is not quite

[7]From the imaginary part the continuity equation (5.1) follows.

[8]GRWm stands for GhirardiRiminiWeber theory with a matter density ontology. This is a spontaneous collapse theory, i.e. the wave function collapses according to a stochastic law. For details see [39, 40].

clear at the moment if these proposals are really of physical relevance.

6 Conclusion

In this thesis, we have provided a mathematically rigorous proof that the so-called Newton-Schrödinger equation is the mean field equation for a N-particle system of identical bosons, interacting via gravitational forces, in the limit $N \to \infty$. As discussed in sec. 2 and sec. 3 the respective many-body Schrödinger equation (1.1) which is the starting point for the proof can be derived from semiclassical gravity or directly from general relativity.

Since our proof is based on Grønwall's lemma, we get also error estimates for systems with finite number of particles.

The proof can be generalized to cases with different types of bosons as well as to fermionic systems. The generalization to fermionic systems is however rather difficult and currently not yet possible for all cases. We have nevertheless no doubt that the difficulties are only technical and solvable.

Despite other claims in the literature about the Newton-Schrödinger equation, we are rather convinced that the Newton-Schrödinger equation only makes sense as an effective mean field equation for many-body systems with very large particle numbers. Interpretations in which the Newton-Schrödinger equation is considered to describe systems containing only one or a few particles are argued to be inconsistent.

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Declaration of Authorship

I hereby confirm that I prepared this master thesis independently and on my own, by exclusive reliance on the tools and literature indicated therein.

Munich, 12.07.2016

Aaron Schaal