Research Article

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Nonlinear PDE Models in Semi-relativistic Quantum Physics

Abstract: We present the self-consistent Pauli equation, a semi-relativistic model for charged spin-1/2 particles with self-interaction with the electromagnetic field. The Pauli equation arises as the $O(1/c)$ approximation of the relativistic Dirac equation. The fully relativistic self-consistent model is the Dirac–Maxwell equation where the description of spin and the magnetic field arises naturally. In the non-relativistic setting, the correct self-consistent equation is the Schrödinger–Poisson equation which does not describe spin and the magnetic field and where the self-interaction is with the electric field only. The Schrödinger–Poisson equation also arises as the mean field limit of the $N$-body Schrödinger equation with Coulomb interaction. We propose that the Pauli–Poisson equation arises as the mean field limit $N \to \infty$ of the linear $N$-body Pauli equation with Coulomb interaction where one has to pay extra attention to the fermionic nature of the Pauli equation. We present the semiclassical limit of the Pauli–Poisson equation by the Wigner method to the Vlasov equation with Lorentz force coupled to the Poisson equation which is also consistent with the hierarchy in $1/c$ of the self-consistent Vlasov equation. This is a non-trivial extension of the groundbreaking works by Lions & Paul and Markowich & Mauser, where we need methods like magnetic Lieb–Thirring estimates.

Keywords: Quantum Physics, Mathematical Modeling, Pauli Equation, Semiclassical Limit, Mean Field Limit

MSC 2020: 35Q40, 81Q05

1 Model Hierarchy

Relativistic quantum mechanics is an immensely successful theory giving a correct description of the behavior of particles on the atomic scale moving at high velocities compared to the speed of light. On the other hand, non-relativistic quantum mechanics is centered around the Schrödinger equation which is insufficient when relativistic effects such as spin and the magnetic field arise. In relativistic quantum mechanics, the description of spin arises naturally in the Dirac equation which is the correct equation for particles with spin 1/2, i.e. fermions. Semi-relativistic quantum mechanics is the theory that keeps relativistic corrections up to order $O(1/c)$, and it has been discovered by Wolfgang Pauli in 1927 that the correct semi-relativistic equation describing charged spin-1/2 particles in the electromagnetic field is the Pauli equation which describes spin and magnetic field through the Stern–Gerlach term.

Since charged particles emit radiation, the effect of self-interaction of a charged particle with the electromagnetic field it generates cannot be neglected in a (semi-)relativistic setting. In the fully relativistic regime, this effect is described by the Dirac–Maxwell equation for spin-1/2 particles. Since Maxwell’s equations are relativistic and Lorentz invariant, it is natural to couple them self-consistently to the Dirac equation. In the non-relativistic regime, the Schrödinger–Poisson equation offers a description of the self-interaction with the electric

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field which is given by a Poisson equation for $V^h$ with the particle density $\rho^h$ as a source term. The magnetic field, being a relativistic effect, does not self-interact at the non-relativistic level and neither does spin which is naturally coupled to the magnetic field. In the semi-relativistic regime of $O(1/c)$, the correct self-consistent description is given by the Pauli–Poisswell equation. Here, Maxwell’s equations for the magnetic vector potential $A^{h,c}$ and the electric scalar potential $V^{h,c}$ are replaced by magnetostatic Poisson equations (cf. [11]) with the current density $j^{h,c}$ and the particle density $\rho^{h,c}$ as source terms. This is appropriate when the typical velocity of the system is small compared to the speed of light. The $O(1/c^2)$ approximation of the Dirac equation is the Pauli–Darwin equation [21, 29, 30].

We have the following diagram for the hierarchies of self-consistent models in relativistic quantum mechanics. The horizontal and vertical arrows indicate the semiclassical ($h \to 0$) and non-relativistic ($c \to \infty$) limits, respectively.

\[
\begin{array}{c}
\text{Dirac–Maxwell} \quad h \to 0 \quad \text{rel. Vlasov–Lorentz–Maxwell} \\
\downarrow \\
\text{Pauli–Darwin } O(1/c^2) \quad h \to 0 \quad \text{rel. Vlasov–Lorentz–Darwin } O(1/c^2) \\
\downarrow \\
\text{Pauli–Poisswell } O(1/c) \quad h \to 0 \quad \text{Vlasov–Lorentz–Poisswell } O(1/c) \\
\downarrow \\
\text{Pauli–Poisson} \quad h \to 0 \quad \text{Vlasov–Lorentz–Poisson} \\
\downarrow \\
\text{magn. Schrödinger–Maxwell} \quad h \to 0 \quad \text{Vlasov–Lorentz–Maxwell} \\
\downarrow \\
\text{magn. Schrödinger–Poisson} \quad h \to 0 \quad \text{Vlasov–Lorentz–Poisson} \\
\downarrow \\
\text{Schrödinger–Poisson} \quad h \to 0 \quad \text{Vlasov–Poisson} \\
\end{array}
\]

Note that the abbreviation “rel.” in front of a Vlasov type equation in the diagram indicates that the velocity $v$ in the Vlasov equation is relativistic, i.e.

\[
v(p) = \frac{p}{\sqrt{\frac{|p|^2}{c^2} + 1}},
\]

where $p$ is the dynamic variable. Otherwise, the velocity is non-relativistic, i.e. $v(p) = p$.

### 1.1 Pauli–Poisswell Equation: A Consistent $O(1/c)$ Model

In the fully self-consistent semi-relativistic model where a magnetostatic $O(1/c)$ approximation of Maxwell’s equations is used to self-consistently describe the magnetic field, the magnetic potential $A^{h,c}$ (depending on $h$ and $c$) is coupled to $\Psi^{h,c}$ via three Poisson type equations with the Pauli current density as source term. This yields the Pauli–Poisswell equation for a 2-spinor $\Psi^{h,c} = (\Psi^{h,c}_1, \Psi^{h,c}_2)^T \in (L^2(\mathbb{R}^3, \mathbb{C}))^2$,

\[
\begin{align}
&i\hbar \partial_t \Psi^{h,c} = -\frac{1}{2m} \left( \hbar \nabla - i \frac{q}{c} A^{h,c} \right)^2 \Psi^{h,c} + q V^{h,c} \Psi^{h,c} - \frac{hq}{2mc} (\sigma \cdot B^{h,c}) \Psi^{h,c}, \\
&\Delta V^{h,c} = -\rho^{h,c} = -|\Psi^{h,c}|^2, \\
&\Delta A^{h,c} = -\frac{1}{c} j^{h,c},
\end{align}
\]
where the Pauli current density is given by

\[ j^{h,c}(\psi^{h,c}, A^{h,c}) = \text{Im} \left( \frac{\hbar}{2m} \left( \hbar \nabla - i \frac{q}{c} A^{h,c} \right) \psi^{h,c} \right) + \hbar \nabla \times \left( \frac{\hbar}{2m} \sigma \psi^{h,c} \right), \]

with initial data

\[ \psi^{h,c}(x, 0) = \psi^{h,c}_I(x) \in (L^2(\mathbb{R}^3))^2. \]

Here, \(|\psi^{h,c}|^2 = |\psi^{h,c}_1|^2 + |\psi^{h,c}_2|^2\). Spin and magnetic field are coupled by the Stern–Gerlach term

\[ \sigma \cdot B^{h,c} := \sum_{k=1}^{3} \sigma_k B_k^{h,c}, \]

where \(B^{h,c} = \nabla \times A^{h,c}\) is the magnetic field and where the \(\sigma_k\) are the Pauli matrices

\[
\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\]

The Pauli–Poisson equation is the only consistent \(O(1/c)\) approximation of the Dirac–Maxwell equation. It was derived in [28]. The two components of the Pauli equation describe the two spin states of a fermion, whereas the Poisson equations describe the electrodynamic self-interaction of a fast moving particle with the electromagnetic field that it generates itself due to the finite speed of light. Since \(A^{h,c}\) is coupled to \(\psi^{h,c}\), we write a superscript \(h, c\) in order to emphasize its dependence on the semiclassical and the relativistic parameter. Compare (1.4) to (1.8) and notice that, in the former, the magnetic potential depends on \(h\) and \(c\). The semiclassical limit of (1.1)–(1.3) to the Vlasov equation with Lorentz force coupled to the Poisson equations (Vlasov–Poisson equation) by the Wigner method is to be published in [32]. The numerics of the Vlasov–Poisson equation were discussed in [11]. The existence of classical solutions was discussed in [39]. The classical limit \(c \to \infty, h \to 0\) of the Dirac–Maxwell equation to the Vlasov–Poisson equation was proven in [33] where the authors first perform the non-relativistic limit to the Schrödinger–Poisson equation and then the semiclassical limit to the Vlasov–Poisson equation. The semiclassical limit of the Dirac–Maxwell equation to the relativistic Vlasov–Maxwell equation is a very hard open question. We would like to mention two recent works on the regularity of weak solutions to the Vlasov–Maxwell equation by Besse & Bechouche [10] and Bardos, Besse & Nguyen [4].

### 1.2 Pauli–Poisson and Magnetic Schrödinger–Maxwell Equation

In the situation where an external magnetic field \(A\) is applied which is much stronger than the self-consistent magnetic field generated by the particle, then the appropriate model is the Pauli–Poisson equation given by

\[ i\hbar \partial_t \psi^{h,c} = -\frac{1}{2m} \left( \hbar \nabla - i \frac{q}{c} A \right)^2 \psi^{h,c} + q V^{h,c} \psi^{h,c} - \frac{\hbar q}{2cm} (\sigma \cdot B) \psi^{h,c}, \]

\[ \Delta \psi^{h,c} = -\rho^{h,c} := -|\psi^{h,c}|^2, \]

with initial data

\[ \psi^{h,c}(x, 0) = \psi^{h,c}_I(x) \in (L^2(\mathbb{R}^3))^2. \]

and Pauli current density \(j^{h,c}\) given by

\[ j^{h,c} = \text{Im} \left( \frac{\hbar}{2m} \left( \hbar \nabla - i \frac{q}{c} A \right) \psi^{h,c} \right) + \hbar \nabla \times \left( \frac{\hbar}{2m} \sigma \psi^{h,c} \right). \]

More generally, we may consider the Pauli–Hartree equation

\[ i\hbar \partial_t \psi^{h,c} = -\frac{1}{2m} \left( \hbar \nabla - i \frac{q}{c} A \right)^2 \psi^{h,c} + V^{\text{ext}} \psi^{h,c} - \frac{\hbar q}{2cm} (\sigma \cdot B) \psi^{h,c} + (W \ast |\psi^{h,c}|^2) \psi^{h,c}, \]

where \(V^{\text{ext}}\) is an external potential and \(W\) is an interaction kernel depending on \(x \in \mathbb{R}^3\). In three dimensions only, the Pauli–Poisson equation corresponds to the Pauli–Hartree equation with

\[ W(x) = -\frac{\lambda}{|x|^4}, \]
where $\lambda$ is a coupling constant. The Pauli–Poisson equation is related to the magnetic Schrödinger–Maxwell equation, considered in [8], the magnetic Schrödinger–Poisson equation, considered in [2, 3], and the magnetic Schrödinger–Hartree equation, considered in [26, 34].

The Pauli–Poisson, magnetic Schrödinger–Maxwell and magnetic Schrödinger–Poisson equations are all inconsistent models in the small parameter $1/c$. In fact, these models omit terms of order $O(1/c)$ and are therefore $O(1)$ in $1/c$. The magnetic Schrödinger–Maxwell equation in Lorenz gauge is given by

$$i\hbar \partial_t \psi^h = -\frac{1}{2m} \left( \hbar \nabla - i \frac{q}{c} A^h \right)^2 \psi^h + q V^h \psi^h, \quad \Box V^h = 4\pi |\psi^h|^2, \quad \Box A^h = \frac{4\pi}{c} j^h,$$

where

$$j^h = \text{Im} \left( \overline{\psi^h} \left( \hbar \nabla - i \frac{q}{c} A^h \right) \psi^h \right)$$

(1.9)
is the current density of the magnetic Schrödinger equation and initial data

$$\psi^h(x, 0) = \psi_0^h, \quad A^h(x, 0) = a_0^h, \quad \partial_t A^h(x, 0) = a_1^h.$$

The magnetic Schrödinger–Poisson equation is given by

$$i\hbar \partial_t \psi^h = -\frac{1}{2m} \left( \hbar \nabla - i \frac{q}{c} A^h \right)^2 \psi^h + q V^h \psi^h, \quad \Box V^h = -|\psi^h|^2,$$

(1.10)

with initial data

$$\psi^h(x, 0) = \psi_0^h(x) \in L^2(\mathbb{R}^3),$$

(1.12)

The magnetic Schrödinger–Hartree equation is given by

$$i\hbar \partial_t \psi^h = -\frac{1}{2m} \left( \hbar \nabla - i \frac{q}{c} A^h \right)^2 \psi^h + V_{\text{ext}} \psi^h + (W * |\psi^h|^2) \psi^h,$$

(1.13)

with initial data

$$\psi^h(x, 0) = \psi_0^h(x) \in L^2(\mathbb{R}^3),$$

(1.14)

In $\mathbb{R}^3$ with $W(x) \sim |x|^{-1}$, we obtain the magnetic Schrödinger–Poisson equation (1.10)–(1.12) from the magnetic Schrödinger–Hartree equation. Here, we use a lower case $\psi^h$ to denote a scalar wave function. Compare (1.9) to (1.8) where we have an additional divergence-free term due to the spin coupling which is not present in (1.9).

In [2, 3], the global wellposedness for bounded external potentials was shown. In [26], the mean field limit of the $N$-body magnetic Schrödinger equation to the 1-body magnetic Schrödinger–Hartree equation was proved, and in [34], the global wellposedness of the magnetic Schrödinger–Hartree equation for non-Strichartz magnetic field was discussed. The global wellposedness and semiclassical limit of the Pauli–Poisson equation was discussed in [35].

### 1.3 $N$-Body Pauli Equation

Nonlinear 1-body PDEs like the Schrödinger–Poisson equation arise as the mean field limit of linear $N$-body equations with interaction between the particles like the $N$-body Schrödinger equation with Coulomb interaction. A quantum system consisting of a large number $N$ of interacting particles is described by an $N$-body wave function

$$\psi^h_N = \psi^h_N(x_1, \ldots, x_N),$$

where $x_j \in \mathbb{R}^3$. The wave function is normalized in $L^2(\mathbb{R}^{3N})$, i.e.

$$\int_{\mathbb{R}^{3N}} |\psi^h_N(x_1, \ldots, x_N)|^2 \, dx_1 \cdots dx_N = 1,$$
and satisfies the linear $N$-body non-relativistic Schrödinger equation

$$ih\partial_t \psi^h_N = H^h_N \psi^h_N,$$

(1.15)

where $H^h_N$ is the $N$-body Hamiltonian given by

$$H^h_N = -\frac{\hbar^2}{2m} \sum_{j=1}^N \Delta_{x_j} + \frac{1}{N} \sum_{j<k}^N V(|x_j - x_k|),$$

(1.16)

where $V$ is some interaction potential. For the Coulomb interaction, one has $V(x) = |x|^{-1}$, and for the “contact interaction”, $V(x) = \delta(x)$, which results in the Gross–Pitaevskii equation. For large $N$, equation (1.15) becomes impossible to solve numerically. Therefore, it is imperative to approximate linear $N$-body equations by (systems of) nonlinear 1-body equations. The following diagram represents the asymptotic links between $N$-body linear and 1-body nonlinear equations.

The Hartree ansatz for boson condensate, i.e. particles with symmetric $N$-body wave function, is to assume that the initial data are factorized with the same wave function for all bosons,

$$\psi^h_N(x_1, \ldots, x_N, t = 0) = \prod_{j=1}^N \psi^h_I(x_j),$$

which produces a symmetric wave function. This is valid for a pure state of a boson ensemble (i.e. if the system of bosons is in a condensed state). Note that the general Hartree ansatz for bosons would use different orbitals $\psi^h_I$.

For fermions (i.e. for antisymmetric wave functions), a different ansatz has to be chosen. The Hartree–Fock ansatz consists of taking initial fermionic, i.e. antisymmetric $N$-body wave functions $\psi^h_{N,I} \in L^2(S^1)$ (the subspace of $L^2$ consisting of antisymmetric (with respect to permutation of the arguments) wave functions) which give rise to an $N$-body Schrödinger evolution

$$\psi^h_N(x_1, \ldots, x_N, t) = \exp(-iH^h_N t/\hbar) \psi^h_{N,I}(x_1, \ldots, x_N),$$

where $H^h_N$ is the $N$-body Schrödinger Hamiltonian (1.16). The associated initial (pure state) one-particle reduced density matrix $\rho^h_{N,I} \in L^2(\mathbb{R}^{3N})$ (the subspace of $L^2(\mathbb{R}^{3N})$ consisting of antisymmetric with respect to permutation of the arguments) wave functions) which give rise to an $N$-body Schrödinger evolution

$$\psi^h_I(x_1, \ldots, x_N, t) = \frac{1}{\sqrt{N!}} \det(\psi^h_I(x_j, t)),$$

where $\{\psi^h_I\}_{I=1}^N$ is an orthonormal system in $L^2(\mathbb{R}^3)$. The Slater determinant is a particular choice of an antisymmetric wave function. Then $\rho^h_{N,I} \in L^2(\mathbb{R}^{3N})$ should satisfy

$$\text{tr}(\rho^h_{N,I} - \rho^h_{S,I}) \leq C$$

uniformly in $N$. The (pure state) time evolution $\rho^h_S(t)$ of $\rho^h_S(0) = \rho^h_S(0)$ is given by

$$\rho^h_S(t) = \sum_{j=1}^N |\psi^h_J(t)\rangle \langle \psi^h_I(t)|$$

and satisfies the time-dependent Hartree–Fock (TDHF) equation

$$ih\partial_t \rho^h_S(t) = \left[ -\frac{\hbar^2}{2} \Delta + \frac{1}{|x|} \ast \rho^h_{S,\text{diag}}(t) - X, \rho^h_S(t) \right],$$

where $X$ is a self-consistent potential.
where
\[ \rho_{S,\text{diag}}^\hbar(x) = \frac{1}{N} \hat{\rho}^\hbar_{S}(x,x) \]
is the density of \( \hat{\rho}^\hbar_{S} \) and \( X \) denotes the exchange term with integral kernel
\[ X(x,y) = \frac{1}{N} \frac{1}{|x-y|} \hat{\rho}^\hbar_{S}(x,y). \]

It is then expected that the time evolution \( \rho_{N,I}^{\hbar(1)}(t) \) of the initial one-particle reduced density matrix \( \rho_{N,I}^{\hbar(1)} \) should remain close to \( \rho_{S}^{\hbar}(t) \) and their distance in trace norm should vanish in the limit \( N \to \infty \).

The Pauli–Poisson equation should arise as the mean field limit of the \( N \)-body Pauli equation given by
\[ i\hbar \partial_t \Psi_{N}^\hbar = H_{N}^{P} \Psi_{N}^\hbar, \]
where \( H_{N}^{P} \) is the linear \( N \)-body Pauli Hamiltonian with Coulomb interaction given by
\[ H_{N}^{P} = -\frac{1}{2m} \sum_{j=1}^{N} \left( \hbar \nabla_{x_{j}} - \frac{\mu}{c} A(x_{j}) \right)^{2} - \frac{\hbar q}{2cm} (\sigma \cdot B(x_{j})) + \frac{1}{N} \sum_{j<k} \frac{1}{|x_{j} - x_{k}|}, \]
with initial data
\[ \Psi_{N,I}^\hbar = (\Psi_{I}^\hbar)^{\otimes N} \in (L^{2}(\mathbb{R}^{3}))^{\otimes N} \equiv (L^{2}(\mathbb{R}^{3N}))^{2}. \]

The following diagram should hold for the Pauli equation.

Since the Pauli equation holds for fermions, the Pauli exclusion principle implies that the Hartree ansatz as for the bosonic \( N \)-body magnetic Schrödinger equation is in fact not accurate. The correct ansatz is the Hartree–Fock ansatz. However, in practice, the Hartree interaction is sufficient for numerics since the exchange term \( X \) is small in most situations. In fact, the Schrödinger–Poisson–Xα equation was proposed in [31] and studied numerically in [1]. The exchange term \( X \) is replaced by a \( (\hbar)^{2/3}\psi^{H} \), based on an approximation of the exchange term due to Slater [41].

### 2 Asymptotic Analysis

In this section, we emphasize the dependence on \( \hbar \) and \( N \) and use a scaling where \( m = c = q = 1 \). The dependence on \( c \) can be omitted since we only deal with the semiclassical and mean field limits and not with the non-relativistic limit.

#### 2.1 Semiclassical Limit

Mixed states in quantum mechanics represent a statistical ensemble of possible states and are the fundamental object of quantum mechanics since a pure state is a special case of a mixed state. The mixed state formulation is necessary from a technical point of view when dealing with the semiclassical limit of the Schrödinger–Poisson and Pauli–Poisson equations since uniform \( L^{2} \) estimates for the Wigner transform are only possible in a mixed state formulation. A mixed state is represented by a density matrix which is defined as follows.
Let $\{\psi_j^\pm\}_{j \in \mathbb{Z}}$, $\psi_j^h = (\psi_j^h, \psi_j^h)^T$ be an orthonormal system in $(L^2(\mathbb{R}^3))^2$. We define the density matrix $\rho^h$ and the matrix-valued density matrix $R^h$ as

$$
\rho^h(x, y, t) := \sum_{j=1}^{\infty} \lambda_j^h (\psi_{j,1}^h(x, t) \psi_{j,1}^h(y, t)^* + \psi_{j,2}^h(x, t) \psi_{j,2}^h(y, t)^*),
$$

$$
R^h(x, y, t) := \sum_{j=1}^{\infty} \lambda_j^h \psi_{j}^h(x, t) \otimes \psi_{j}^h(y, t),
$$

where $\lambda = \{\lambda_j^h\}_{j \in \mathbb{N}}$ is a normally convergent series such that $\lambda_j^h \geq 0$ and $\sum_j \lambda_j^h = 1$. If there is a $k$ such that $\lambda_j^h = 1$ for $j = k$ and $\lambda_j^h = 0$ otherwise, it represents a mixed state. The density matrix $\rho^h$ can be considered as the kernel of a Hilbert–Schmidt, hermitian, positive and trace class operator $\rho^h$ on $L^2(\mathbb{R}^3)$, called density operator. The diagonal of $\rho^h(x, y)$ corresponds to the particle density and is defined by

$$
\rho^h_{\text{diag}}(x) := \rho^h(x, x) = \sum_{j=1}^{\infty} \lambda_j^h |\psi_{j}^h(x)|^2 \in L^1(\mathbb{R}^3),
$$

$$
R^h_{\text{diag}}(x) := R^h(x, x).
$$

The time evolution of $\rho^h$ is given by the von Neumann equation

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

The Wigner transform $f^h(x, \xi, t)$ and Wigner matrix $F^h$ of $\rho^h$ and $R^h$, respectively, are defined as (cf. [17])

$$
f^h(x, \xi, t) := \frac{1}{(2\pi \hbar)^3} \int_{\mathbb{R}^3} e^{-i\xi y} \rho^h \left( x + \frac{\hbar y}{2}, x - \frac{\hbar y}{2}, t \right) dy,
$$

$$
F^h(x, \xi, t) := \frac{1}{(2\pi \hbar)^3} \int_{\mathbb{R}^3} e^{-i\xi y} R^h \left( x + \frac{\hbar y}{2}, x - \frac{\hbar y}{2}, t \right) dy.
$$

Note that $f^h = \text{Tr}(f^h)$ and $\rho^h = \text{Tr}(R^h)$, where Tr denotes the $2 \times 2$ matrix trace. A simple calculation shows that

$$
\rho^h_{\text{diag}}(x) = \int_{\mathbb{R}^3} f^h(x, \xi) d\xi, \quad R^h_{\text{diag}}(x) = \int_{\mathbb{R}^3} F^h(x, \xi) d\xi.
$$

The mixed state Pauli–Poisson equation is given by

$$
i\hbar \partial_t \psi_j^h = -\frac{1}{2} (\hbar \nabla - iA)^2 \psi_j^h + V \psi_j^h - \frac{1}{2} \hbar (\sigma \cdot B) \psi_j^h,
$$

$$
-\Delta \psi_j^h = \sum_{j=1}^{\infty} \lambda_j^h |\psi_j^h|^2 = \rho^h_{\text{diag}},
$$

$$
\psi_j^h(x, 0) = \psi_j^h(x) \in (L^2(\mathbb{R}^3))^2,
$$

where the mixed state Pauli current density is given by

$$
f^h(\psi^h, A) = \sum_{j=1}^{\infty} \lambda_j^h \left[ \text{Im} \left( \overline{\psi_j^h} (\hbar \nabla - iA) \psi_j^h \right) - \hbar \nabla \times (\overline{\psi_j^h} \sigma \psi_j^h) \right],
$$

Rewriting (2.1)–(2.3) in the density matrix formulation using the von Neumann equation and taking its Wigner transform, one obtains the Pauli–Wigner–Poisson equation for $F^h$,

$$
\partial_t F^h + \xi \cdot \nabla x F^h - [\nabla_j [\beta[A]] \ast_x \nabla_t F^h - \theta[A](\xi F^h)
+ \frac{1}{2} \theta[A]^2 \partial_t F^h - \frac{\hbar}{2} \theta[A] \sigma \cdot B F^h + \theta[V] F^h = 0,
$$

$$
-\Delta V^h = \rho^h_{\text{diag}} = \int_{\mathbb{R}^3} f^h d\xi,
$$

$$
F^h(x, \xi, 0) = F^h_0(x, \xi),
$$
We easily obtain, after a change of variables

where

\int \delta \cdot |(x, y, t) \Phi^h(x, \eta, t) e^{-i(\xi - \eta) \cdot y} \, d \eta \, dy,

where

\begin{align*}
\beta[g] & := \frac{1}{2} \left( g \left( x + \frac{hy}{2} \right) + g \left( x - \frac{hy}{2} \right) \right), \\
\delta[g] & := \frac{i}{\hbar} \left( g \left( x + \frac{hy}{2} \right) - g \left( x - \frac{hy}{2} \right) \right).
\end{align*}

Under suitable assumptions on the potentials and the initial data which are listed in Assumption 1 and in

\begin{align*}
\text{Theorem 1}, \text{equations (2.4)} & \text{– (2.6) converge to}
\partial_t F + \xi \cdot \nabla_x F - A \cdot \nabla_x F + (\nabla_x A) \xi \cdot \nabla_x F - \nabla_x F \cdot \nabla_x F - \nabla_x V(x) \cdot \nabla_x F = 0, \\
-\Delta V & = \rho_{\text{diag}} = \int f \, d \xi, \\
F(x, \xi, 0) & = F_1(x, \xi),
\end{align*}

where \( f := \text{Tr}(F) \). As expected, the Stern–Gerlach term \( h \theta(\sigma \cdot B) F^h \) converges to zero in the semiclassical limit. We easily obtain, after a change of variables \( p = \xi - A \) and by using \( B = \nabla \times A \),

\begin{align*}
\partial_t F + p \cdot \nabla_x F + (-\nabla_x V + p \times B) \cdot \nabla_p F = 0,
\end{align*}

which is the magnetic Vlasov equation with Lorentz force for an electron.

**Assumption 1.** Let \( R^h \) or \( \rho^h \) be a matrix-valued density matrix or density matrix defined by an orthonormal system \( \{ \Psi_j^h \} \subset (L^2(\mathbb{R}^3))^2 \) and occupation probabilities \( \lambda_j^h \in [0, 1] \). We assume that

\begin{align*}
\lambda_j^h & \geq 0, \quad \sum_{j=1}^\infty \lambda_j^h = 1, \\
\frac{1}{\hbar^3} \sum_{j=1}^\infty (\lambda_j^h)^2 & = \frac{1}{\hbar^3} \| \lambda^h \|_2^2 \leq C. \tag{2.7}
\end{align*}

Since (2.7) implies that the sequence \( \{ \lambda^h \} \) depends on \( h \), the reason for the superscript becomes apparent. This assumption implies uniform \( L^2 \) bounds in \( h \) for the Wigner transform.

We have the following theorem from [35].

**Theorem 1.** Let \( \{ \Psi_j^h \}_{j \in \mathbb{N}} \in C(\mathbb{R}_t, (L^2(\mathbb{R}^3))^2) \) be a solution of the mixed state Pauli–Poisson equation (2.1)–(2.3) with associated matrix-valued density matrix \( \rho^h \) such that the occupation probabilities satisfy Assumption 1. Let \( F^h \) be the associated Wigner matrix solving the Pauli–Wigner equation (2.4) with initial data \( F^h_1(x, p) = F^h(x, p, 0) \). Assume \( F^h \) converges up to a subsequence in \( S'((\mathbb{R}^3 \times \mathbb{R}_p)^{2 \times 2}) \) to a nonnegative matrix-valued Radon measure \( F_1 \).

(i) Let \( A, V \in C^1(\mathbb{R}^3) \) such that \( B := \nabla \times A \in C(\mathbb{R}^3) \). Then \( F^h \) converges weakly* up to a subsequence in \( (S')^{2 \times 2} \) to \( F \in C_0(\mathbb{R}_t, \mathcal{M}_{\text{w}}^{(2 \times 2)}) \) such that \( F \) solves the Vlasov–Poisson equation with Lorentz force

\begin{align*}
\partial_t F + p \cdot \nabla_x F + (-\nabla_x V + p \times B) \cdot \nabla_p F = 0
\end{align*}

in \( (\mathbb{R}^3)^{2 \times 2} \) verifying the initial condition

\begin{align*}
F(x, p, 0) = F_1(x, p) \quad \text{in } \mathbb{R}_x^3 \times \mathbb{R}_p^3.
\end{align*}

(ii) Let \( V^h \) be given by \( -\Delta V^h = \rho_{\text{diag}}^h \) and suppose that \( A \in W^{1,1}(\mathbb{R}^3) \). Moreover, suppose that \( \{ F_j^h \} \) is a bounded sequence in \( (L^2(\mathbb{R}^3))^2 \times \mathbb{R}^3 \) and that the initial energy is bounded independently of \( h \). Then \( F^h \) converges weakly* up to a subsequence in \( L^{\infty}(I, L^2(\mathbb{R}_x^3 \times \mathbb{R}_p^3)^{2 \times 2}) \) to

\begin{align*}
F \in C_b(\mathbb{R}_t, \mathcal{M}_{\text{w}}^{(2 \times 2)}) \cap L^{\infty}(I, L^2(\mathbb{R}_x^3 \times \mathbb{R}_p^3)^{2 \times 2})
\end{align*}
such that $F$ solves
\[ \partial_t F + p \cdot \nabla_x F + (-\nabla_x V + p \times B) \cdot \nabla_p F = 0 \]
in $(D')^{2 \times 2}$ and
\[ -\Delta V = \rho_{\text{diag}}(x), \quad \rho_{\text{diag}}(x) = \int f(x, p) \, dp, \]
where $f = \text{Tr}(F)$, verifying the initial condition
\[ F(x, p, 0) = F_I(x, p) \quad \text{in } \mathbb{R}^3 \times \mathbb{R}^3. \]

(iii) Let $A \in W^{1,2}(\mathbb{R}^3)$. The mixed state Pauli current density $J^h$ defined by
\[ J^h = \sum_{j=1}^{\infty} \lambda^h_j \left[ \text{Im}(\overline{\Psi^h_j}(h \nabla - iA)\Psi^h_j) - h\nabla \times (\overline{\Psi^h_j} \sigma \Psi^h_j) \right] \]
converges in $D'$ to
\[ J = \int_{\mathbb{R}^3} p f \, dp. \]

Remark 1. Some remarks about Theorem 1 and its relation to existing results are in order. In 1993, Lions & Paul [24] and Markowich & Mauser [27] independently proved the semiclassical limit of the Schrödinger–Poisson equation to the non-relativistic Vlasov–Poisson equation. Compared to the Pauli–Poisson equation, the 2-spinor $\Psi^h$ is replaced by a scalar wave function $\psi^h$ and $A^h = B^h \equiv 0$.

The main difference to the proof of Theorem 1 is the use of regular Lieb–Thirring estimates which do not involve the magnetic field $B^h$. For Theorem 1, one has to employ magnetic Lieb–Thirring estimates which were obtained in [14] and refined in [40]. The analysis of the Pauli equation is much more complicated than that of the (magnetic) Schrödinger equation because of the existence of zero modes due to the presence of the Stern–Gerlach term involving the magnetic field $B = \nabla \times A$.

Moreover, in the Schrödinger–Poisson case, the associated Wigner equation (i.e. the Wigner–Poisson equation) is much simpler than (2.4). In fact, the only term whose limit has to be justified is the term involving $V^h$.

Remark 2. The importance of a mixed state formulation was already highlighted by Yvon in [43]. He pointed out that a pure state formulation was insufficient for the Wigner formalism, and he showed that the Wigner transform of a density matrix is the unique function which produces the right moments and has the right properties analogous to a classical phase space density.

2.2 Mean Field Limit

For bounded interaction potential, the bosonic $N$-body Schrödinger equation (1.15) was shown in [7, 42] to converge to the Hartree equation
\[ i\hbar \partial_t \psi^h = -\frac{\hbar^2}{2} \psi^h + (V * |\psi^h|^2) \psi^h. \]
This was extended in [5, 15] to the Coulomb potential
\[ V(x) = \frac{\lambda}{|x|}, \]
which implies the convergence of the three-dimensional $N$-body Schrödinger equation with Coulomb interaction to the Schrödinger–Poisson equation.

The convergence of the fermionic $N$-body Schrödinger equation to the TDHF equation was shown for bounded, symmetric binary interaction potentials $V$ (boundedness excludes the Coulomb potential) in [6]. The problem of the convergence of the fermionic $N$-body Schrödinger equation with Coulomb interaction to the Hartree–Fock equation is hard due to the singular nature of the Coulomb potential. The Hartree–Fock dynamics
for Coulomb interaction were proved in [38] for the scaling $h = N^{-1/3}$ which links the mean field limit with the semiclassical limit, in [36] for a different scaling linking potential and kinetic energy and in [16] for the same scaling as in [6]. It is shown that the fermionic $N$-body Schrödinger equation with Coulomb potential is approximated by the Hartree–Fock equation in the sense that the time evolutions stay close in the trace norm. This result holds for $\rho_N^h$ representing a pure state, i.e. $\rho_N^h$ is given by an orthogonal projection on the $N$-dimensional subspace spanned by antisymmetric wave functions. Notice that this is at odds with the semiclassical limit of the Schrödinger–Poisson equation in $\mathbb{R}^3$ to the Vlasov–Poisson equation [24, 27] and the limit of the Pauli–Poisson equation to the Vlasov–Poisson equation with Lorentz force in [35] where only mixed states are allowed since the occupation probabilities have to satisfy condition (2.7) in order for the Wigner transform to be bounded uniformly in $L^2$. A recent result for the Hartree–Fock dynamics of fermionic mixed states is [9]; however, it does not include Coulomb interaction. Moreover, in [38], the assumptions on the initial data for $\rho_N^h$ are restrictive in the sense that one needs control over the commutator $[x, \rho_N^h]$ for which the authors of [38] did not find non-trivial sufficient conditions. For an excellent introduction to the topic, cf. the survey by Golse [18], as well as the result by Pickl [37].

For the bosonic magnetic Schrödinger equation with Coulomb interaction, the $N$-body Hamiltonian is given by

$$H_N^0 = -\frac{1}{2} \sum_{j=1}^{N} (\hbar^2 \nabla_j - i A(x_j))^2 + \frac{1}{N} \sum_{j<k} \frac{1}{|x_j - x_k|}. $$

The $N$-body wave function $\psi_N^h$ satisfies the $N$-body magnetic Schrödinger equation

$$i \hbar \partial_t \psi_N^h = H_N^{0h} \psi_N^h$$

with initial data

$$\psi_{N,0}^h = (\psi_1^h)^{\otimes N} \in L^2(\mathbb{R}^{3N}).$$

The following theorem is due to Lührmann [26] where it is shown that the linear $N$-body magnetic Schrödinger equation with Coulomb interaction converges to the magnetic Schrödinger–Hartree equation in the limit $N \to \infty$ for pure states and for $h$ fixed. The proof is a straightforward combination of a result by Knowles and Pickl [22] and the properties of the magnetic Schrödinger operator. The space $H_0^1$ denotes the magnetic Sobolev space with norm $\|f\|_{H_0^1} = \|f\|_2 + \|(\nabla - iA)f\|_2$.

**Theorem 2 ([26]).** Let $A \in C^{\alpha}$ such that

$$\| \partial^\alpha B(x) \| \leq C_\alpha \frac{1}{(1 + |x|)^{(1+\epsilon)}} \quad \text{for all } |\alpha| \geq 1, x \in \mathbb{R}^3$$

and let $\psi_{N,0}^h := (\psi_1^h)^{\otimes N} \in H_0^1(\mathbb{R}^{3N})$ be initial data to the $N$-body magnetic Schrödinger equation (2.8) such that $\|\psi_{N,0}^h\|_2 = 1$. Let $\rho_N^{h,(k)}$ be the $k$-particle marginal density, where $\rho_N^h = |\psi_N^h\rangle \langle \psi_N^h|$, and let $\psi^h$ be the solution to the magnetic Schrödinger–Hartree equation (1.13) corresponding to the initial data $\psi_1^h$. Then there exists a constant $C > 0$ such that, for $k \in \mathbb{N}$ and $t \in \mathbb{R}$,

$$\text{tr}(\rho_N^{h,(k)} - |\psi^h\rangle \langle \psi^h|)^{1/k} \leq \sqrt{3} \left( \frac{k}{N} e^{Ct} \right)^{1/k} \quad \text{for all } k \leq N.$$

The constant $C$ depends on $\|\psi^h\|_{H_0^1(\mathbb{R}^3)}$. In particular, $\rho_N^{h,(k)}$ converges in trace to $|\psi^h\rangle \langle \psi^h|^{1/k}$ as $N \to \infty$.

### 3 Wellposedness of Pauli–Poisson

In this section, we omit all superscripts since we do not consider asymptotics. We have the following global wellposedness result for the mixed state Pauli–Poisson equation (2.1)–(2.3) from [35]. Here, $\Psi := \{\Psi_j\}_{j \in \mathbb{N}}$ and $\Psi_I = \{\Psi_{I,j}\}_{j \in \mathbb{N}}$. The energy space $\mathcal{H}^1(\mathbb{R}^3)$ is defined as

$$\mathcal{H}^1(\mathbb{R}^3) := \{\Psi \in L^2 : (\nabla - iA)\Psi \in L^2, (\sigma \cdot B)_{+}^{1/2}\Psi \in L^2\}$$

where $\sigma \cdot B_{+}$ is the positive part of the Lorentz force.
with associated norm
\[ \| \Psi \|_{L^2}^2 := \| (V - iA) \Psi \|_2^2 + \| (\sigma \cdot B) \|_2^{1/2} \| \Psi \|_2^2 + \| \Psi \|_2^2. \]

**Theorem 3.** Let \( A \in L^2_{loc}(\mathbb{R}^3), |B| \in L^2(\mathbb{R}^3). \) For any \( \Psi_t \in H^1(\mathbb{R}^3), \) there exists a unique solution to the initial value problem (2.1)–(2.3) in \( C(\mathbb{R}, H^1(\mathbb{R}^3)) \cap C^1(\mathbb{R}, H^1(\mathbb{R}^3)^*) \). If \( \Psi_{n,t} \), \( \Psi_t \in H^1(\mathbb{R}^3) \) are initial data satisfying \( \Psi_{n,t} \to \Psi \) in \( H^1(\mathbb{R}^3) \) with corresponding unique solutions
\[ \Psi_{n,t} \in C(\mathbb{R}, H^1) \cap C^1(\mathbb{R}, H^1) \quad \text{and} \quad \Psi \in C(\mathbb{R}, H^1) \cap C^1(\mathbb{R}, H^1^*), \]
then \( \Psi_{n,t} \to \Psi \) in \( L^\infty(\mathbb{R}, H^1(\mathbb{R}^3)). \)

The global wellposedness in the energy space for the magnetic Schrödinger equation with Hartree nonlinearity \( W \ast |\Psi|^2 \) (including \( W(x) = |x|^{-1} \)) for the pure state case, i.e. (1.13)–(1.14), was proven in [34]. The magnetic Laplacian defines a self-adjoint operator on \( H^1 \). Then one shows that the Hartree nonlinearity is Lipschitz in the energy space, and finally, one uses energy conservation to extend the solution globally. In [34], the magnetic potential \( A \) is assumed to be in \( L^2_{loc}(\mathbb{R}^3) \) which is sufficient for the magnetic Laplacian \( \Delta_A \) to be self-adjoint on \( L^2(\mathbb{R}^3) \) due to a theorem by Leinfelder and Simader; cf. [23].

In [3], wellposedness of the magnetic Schrödinger–Poisson equation is proved for mixed states, but only for bounded magnetic fields. Global wellposedness in \( H^2 \) of the Schrödinger–Poisson equation without magnetic field for mixed states was obtained in [12, 20] and in \( L^2 \) in [13].

We have the following straightforward generalization of Theorem 3 to the Pauli–Hartree equation.

**Theorem 4 (Global Wellposedness of Pauli–Hartree).** Under the assumptions of Theorem 3 and assuming that \( W \) is even, \( W \in L^{r_2}(\mathbb{R}^3) + L^{\infty}(\mathbb{R}^3) \) for \( 3/2 \leq r_1 \leq \infty \) and \( \nabla W \in L^{r_2} + L^{\infty} \) for \( 1 \leq r_2 \leq \infty \), the Pauli–Hartree equation is globally wellposed in \( H^1(\mathbb{R}^3). \)

**Remark 3.** The question arises whether the Pauli–Hartree equation can be posed in arbitrary space dimensions. The three-dimensional magnetic field \( B = \nabla \times A \) has to be replaced by its \( d \)-dimensional generalization \( \nabla \wedge A \). In this case, following the result for the magnetic Schrödinger–Hartree equation [34], the conditions for \( W \) would be the following: \( W \) even, \( W \in L^{r_1}(\mathbb{R}^3) + L^{\infty}(\mathbb{R}^3) \) for \( \max(1, d/2) \leq r_1 \leq \infty \) (\( r_1 > 1 \) if \( d = 2 \)) and \( \nabla W \in L^{r_2} + L^{\infty} \) for \( \max(1, d/3) \leq r_2 \leq \infty \).

Theorems 3 and 4 are novel in the sense that they extend existing results by considering the Pauli operator with the Stern–Gerlach term, mixed states (compared to [34]) and less regular potentials (compared to [3]).

## 4 Numerical Analysis

The numerical analysis of the Pauli equation is not well developed yet. For the linear Pauli equation with given external potentials \( V \) and \( A \), using an operator splitting scheme was studied in [19] where the linear Pauli Hamiltonian
\[ -\Delta + 2iA \cdot \nabla + |A|^2 + V - (\sigma \cdot B) \]
is split into the “kinetic step” \(-\Delta\), the “advection step” \( 2iA \cdot \nabla \), the “potential step” \( |A|^2 + V + \text{diag}(B_3, -B_3) \) and the “coupling step” which consists of the off-diagonal elements of \( \sigma \cdot B \). The most computationally demanding step is the advection step which is solved in [19] by the method of characteristics combined with Fourier interpolation.

The numerical analysis for the Pauli–Poissswell equation is much harder due to the nonlinear coupling of the potentials via the 3 + 1 Poisson equations. Since, already in the linear Pauli equation, the advection step is the most complicated one, the fact that, in the Pauli–Poissonwells equation, \( A \) is given by the Poisson equation with the current density as source term will require more sophisticated methods for the numerical analysis.

For the non-magnetic case without spin, i.e. the Schrödinger–Poisson equation, Lubich proved stability of an operator splitting in [25]. The first step for the numerical analysis of the Pauli–Poissonwells equation could be to generalize this result to the magnetic Schrödinger–Poisson equation and then to the Pauli–Poisson equation by adding the spin term.
5 Conclusion

The Pauli–Poisson equation (1.5)–(1.8) offers an improved model over the existing magnetic Schrödinger–Poisson and magnetic Schrödinger–Hartree equations since it includes the description of spin and the magnetic field. It is not a fully self-consistent model since the magnetic field is considered an external effect. However, the model can be further justified as the mean field limit of the $N$-body Pauli equation with Coulomb interaction. Future work will have to make this statement rigorous.

The semiclassical analysis of the Pauli–Poisson equation by the Wigner method in [35] is the first novel result in the direction of the semiclassical limit of the Dirac–Maxwell equation since the works by Lions & Paul [24] and Markowich & Mauser [27]. The semiclassical analysis of the fully self-consistent Pauli–Poisswell equation is much harder due to the nonlinear coupling of the Pauli current and will be addressed in future publications.

The numerical analysis is still open and will be worked out based on carefully chosen operator splitting techniques. Again, the Pauli–Poisson equation will be significantly easier than the analysis of the Pauli–Poisswell equation.

**Funding:** We acknowledge support from the Austrian Science Fund (FWF) via the grants SFB F65 and W1245 and by the Vienna Science and Technology Fund (WWTF) project MA16-066 “SEQUEX”.

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