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Derivation of the Schrödinger–Poisson equation from the quantum N-body problem

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Abstract We derive the time-dependent Schrödinger–Poisson equation as the weak coupling limit of the N-body linear Schrödinger equation with Coulomb potential. ***To cite this article: C. Bardos et al., C. R. Acad. Sci. Paris, Ser. I 334 (2002) 515–520.*** © 2002 Académie des sciences/Éditions scientifiques et médicales Elsevier SAS

Justification de l'équation de Schrödinger–Poisson à partir du problème quantique à N corps

Résumé On établit la validité de l'équation de Schrödinger–Poisson en régime instationnaire comme limite à couplage faible de l'équation de Schrödinger linéaire à N corps avec potentiel de Coulomb. ***Pour citer cet article : C. Bardos et al., C. R. Acad. Sci. Paris, Ser. I 334 (2002) 515–520.*** © 2002 Académie des sciences/Éditions scientifiques et médicales Elsevier SAS

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Considérons un système de N particules chargées de masse m et de charge q dont l'évolution est gouvernée par l'équation de Schrödinger linéaire à N-corps :

$$i\hbar\partial_t\Psi_N = -\frac{\hbar^2}{2m}\sum_{k=1}^{N}\Delta_{x_k}\Psi_N + q^2\sum_{1\leqslant k<l\leqslant N} V\left(|x_k-x_l|\right)\Psi_N, \quad x_1,\dots,x_N\in\mathbf{R}^3. \tag{1}$$

L'inconnue $\Psi_N \equiv \Psi_N(t,x_1,\dots,x_N)$ est appelée « fonction d'onde à N corps » et le modèle (1) est considéré comme exact en mécanique quantique non relativiste.

Compte tenu du très grand nombre de particules intervenant en pratique, on cherche à approcher cette description exacte par un modèle non linéaire de champ moyen pour une fonction d'onde à 1 corps $\Psi \equiv \Psi(t,x)$. L'exemple le plus simple de cette approximation consiste à supposer $\Psi_{N|t=0}$ factorisée, c'est à

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dire de la forme $\Psi_N(0, x_1, \ldots, x_N) = \prod_{k=1}^N \Psi(0, x_k)$ et que, pour tout $t > 0$, Ψ est gouvernée par l'équation de Hartree :

$$i\hbar\partial_t \Psi(t,x) = -\frac{\hbar^2}{2m}\Delta_x \Psi(t,x) + \left(q^2 \int V\left(|x-y|\right)\left|\Psi(t,y)\right|^2 \mathrm{d}y\right)\Psi(t,x), \quad x \in \mathbf{R}^3. \tag{2}$$

Dans le cas d'une interaction coulombienne $V(r) = 1/r$ dans (1) et (2) et l'équation de Hartree (2) est appelée « équation de Schrödinger–Poisson ».

Spohn avait donné une démonstration de l'approximation de Hartree dans le seul cas où le potentiel V est borné : voir [10]. Nous étendons ici son résultat à une classe très large de potentiels V contenant en particulier le cas du potentiel coulombien.

Notre preuve est basée sur des estimations a priori uniformes en N portant sur la hiérarchie de BBGKY quantique garantissant l'unicité de la solution pour le problème limite par un argument de type Cauchy–Kowalewski. Nous renvoyons à [1] et [3] pour une version détaillée de ces démonstrations.

1. Introduction

Consider a large number N of particles of like mass m and charge q coupled by a radial (real-valued) potential V. In nonrelativistic quantum mechanics, the first principle model governing the evolution of such a system is the linear Schrödinger equation (1) for the N-body wave function $\Psi_N \equiv \Psi_N(t, x_1, \ldots, x_N)$.

In most realistic situations, the number N is so large that one seeks to approximate the exact model (1) by a nonlinear mean field equation for a 1-particle wave function $\Psi \equiv \Psi(t,x)$. A standard way of doing this is to postulate that $\Psi_{N|t=0}$ is of the form $\Psi_N(0, x_1, \ldots, x_N) = \prod_{k=1}^N \Psi(0, x_k)$ and that Ψ solves the Hartree equation (2) for all $t > 0$, this ansatz corresponding to the case where the particles considered are bosons.

The goal of this note is to provide a mathematical derivation of the approximate mean-field equation (2) from the first principle model (1) under some appropriate scaling assumption as $N \to \infty$. A derivation for bounded Vs was given by Spohn [10], in second quantized formalism by Hepp [4], and for singular potential by Ginibre and Velo [5]. The last approach requires special initial states with no definite particle numbers. The method described below allows to consider more general potentials, especially the Coulomb potentials $V(r) = 1/r$ of paramount importance for applications to atomic physics, in which case (2) is referred to as the Schrödinger–Poisson equation.

2. Compactness properties and existence theory for hierarchies

Below, we choose to work with density matrices rather than with wave functions. To a wave function $\Psi_N(t, x_1, \ldots, x_N) \in \mathbf{C}$ is associated the density matrix

$$\rho_N(t, x_1, \ldots, x_N, y_1, \ldots, y_N) = \Psi_N(t, x_1, \ldots, x_N)\overline{\Psi_N(t, y_1, \ldots, y_N)}. \tag{3}$$

Since the quantum particles under consideration are indistinguishable,

$$\rho_N(t, x_{\sigma(1)}, \ldots, x_{\sigma(N)}, y_{\sigma(1)}, \ldots, y_{\sigma(N)}) = \rho_N(t, x_1, \ldots, x_N, y_1, \ldots, y_N) \tag{4}$$

for any permutation $\sigma \in \mathfrak{S}_N$. In the sequel, we denote for any n such that $1 \leqslant n \leqslant N$, $X_n = (x_1, \ldots, x_n)$ while, if $1 \leqslant n < N$, $X_N^n = (x_{n+1}, \ldots, x_N)$. The wave function Ψ_N is normalized by the relation

$$\int \left|\Psi_N(t, X_N)\right|^2 \mathrm{d}X_N = 1, \quad t \in \mathbf{R}. \tag{5}$$

Both conditions (4) and (5) are propagated by the Schrödinger equation (1). We consider this Schrödinger equation (1) in dimensionless variables chosen so that

$$
\begin{aligned}
i\partial_t \Psi_N = \mathcal{H}_N \Psi_N \;&:=\; -\frac{1}{2}\sum_{k=1}^{N} \Delta_{x_k}\Psi_N + \frac{1}{N}\sum_{1\leqslant k<l\leqslant N} V\big(|x_k-x_l|\big)\Psi_N, \quad t\in\mathbf{R},\ X_N\in\big(\mathbf{R}^3\big)^N;\\
\Psi_N(0,X_N) \;&=\; \Psi_N^{\mathrm{in}}(X_N), \quad X_N\in\big(\mathbf{R}^3\big)^N.
\end{aligned}
\tag{6}
$$

The $1/N$ factor in front of the potential energy characterizes the so-called "weak-coupling scaling" under which the mean-field limit described above can be established.

The object of interest is the sequence of n-marginals of the N-body density matrix (3) defined by

$$
\rho_{N,n}(t,X_n,Y_n) = \int \rho_N\big(t,X_n,Z_N^n,Y_n,Z_N^n\big)\,\mathrm{d}Z_N^n, \quad 1\leqslant n<N, \quad \rho_{N,N}=\rho_N, \quad \rho_{N,n}=0, \quad n>N.
\tag{7}
$$

They satisfy the "N-body Schrödinger hierarchy"

$$
\begin{aligned}
i\partial_t \rho_{N,n}(t,X_n,Y_n) \;=\; &-\frac{1}{2}(\Delta_{X_n}-\Delta_{Y_n})\rho_{N,n}(t,X_n,Y_n) + \frac{N-n}{N}(\mathcal{C}_{n,n+1}\rho_{N,n+1})(t,X_n,Y_n)\\
&+\frac{1}{N}\sum_{1\leqslant k<l\leqslant n}\big[V\big(|x_k-x_l|\big)-V\big(|y_k-y_l|\big)\big]\rho_{N,n}(t,X_n,Y_n), \quad 1\leqslant n<N,
\end{aligned}
\tag{8}
$$

where the operator $\mathcal{C}_{n,n+1}$ is defined by

$$
(\mathcal{C}_{n,n+1}\rho_{N,n+1})(t,X_n,Y_n) = \sum_{k=1}^{n}\int\big[V\big(|x_k-z|\big)-V\big(|y_k-z|\big)\big]\rho_{N,n+1}(t,X_n,z,Y_n,z)\,\mathrm{d}z.
\tag{9}
$$

Taking limits formally in (8) (with n fixed and $N\to+\infty$) leads to the "infinite Schrödinger hierarchy"

$$
i\partial_t\rho_n(t,X_n,Y_n) = -\frac{1}{2}(\Delta_{X_n}-\Delta_{Y_n})\rho_n(t,X_n,Y_n) + (\mathcal{C}_{n,n+1}\rho_{n+1})(t,X_n,Y_n), \quad n\geqslant 1.
\tag{10}
$$

This limiting procedure is justified by the following theorem. Before stating it, observe that the normalization (5) allows one to identify $\rho_{N,n}$ with the integral operator

$$
\phi\equiv\phi(X_n)\mapsto\int\rho_{N,n}(t,X_n,Y_n)\phi(Y_n)\,\mathrm{d}Y_n.
$$

This operator belongs to $\mathrm{L}^\infty(\mathbf{R}_+;\mathcal{L}^1(\mathrm{L}^2(\mathbf{R}^{3n})))$, where $\mathcal{L}^1(\mathrm{L}^2(\mathbf{R}^{3n}))$ is the ideal of trace-class operators on the Hilbert space $\mathrm{L}^2(\mathbf{R}^{3n})$. We recall that the weak-* topology on $\mathrm{L}^\infty(\mathbf{R}_+;\mathcal{L}^1(\mathrm{L}^2(\mathbf{R}^{3n})))$ is defined by the family of semi-norms

$$
T\mapsto\left|\int_0^{+\infty}\mathrm{trace}\big(K(t)T(t)\big)\,\mathrm{d}t\right|,
$$

where K runs through $\mathrm{L}^1(\mathbf{R}_+;\mathcal{K}(\mathrm{L}^2(\mathbf{R}^{3n})))$ (the notation $\mathcal{K}(\mathrm{L}^2(\mathbf{R}^{3n}))$ designating the algebra of compact operators on $\mathrm{L}^2(\mathbf{R}^{3n})$). The following theorem is proved in [1] (*see* also [2]).

THEOREM 2.1. – *Assume that* $x\mapsto V(|x|)$ *is bounded from below, belongs to* $\mathrm{C}(\mathbf{R}^3\setminus\{0\})\cap\mathrm{L}^2_{\mathrm{loc}}(\mathbf{R}^3)$ *and satisfies* $\lim_{r\to+\infty}V(r)=0$. *Pick a sequence* Ψ_N^{in} *of initial data that satisfy the normalization of mass* (5) *and of energy*

$$
\mathcal{E}_N = \frac{1}{2}\sum_{k=1}^{N}\int\big|\mathrm{grad}_{x_k}\Psi_N^{\mathrm{in}}(X_N)\big|^2\,\mathrm{d}X_N + \frac{1}{N}\sum_{1\leqslant k<l\leqslant N}V\big(|x_k-x_l|\big)\big|\Psi_N^{\mathrm{in}}(X_N)\big|^2\,\mathrm{d}X_N \leqslant CN
\tag{11}
$$

for some constant $C > 0$, and the condition (4). *The sequence Ψ_N^{in} is further assumed to satisfy*

$$\int \Psi_N^{\text{in}}\big(X_n, Z_N^n, Y_n, Z_N^n\big)\,\mathrm{d}Z_N^n \to \rho_n^{\text{in}}(X_n, Y_n) \tag{12}$$

in $\mathcal{L}^1(\mathrm{L}^2(\mathbf{R}^{3n}))$ weak- for all $n \geqslant 1$. Let Ψ_N be the solution of* (6) *with initial data Ψ_N^{in}* (see [7]). *Then any limit point as $N \to \infty$ in $\prod_{n\geqslant 1}\mathrm{L}^\infty(\mathbf{R}_+; \mathcal{L}^1(\mathrm{L}^2(\mathbf{R}^{3n})))$ weak-* of the sequence $(\rho_{N,n})_{n\geqslant 1}$ defined by* (7) *solves the infinite Schrödinger hierarchy* (10) *with initial data $(\rho_n^{\text{in}})_{n\geqslant 1}$ in the sense of distributions.*

3. An abstract uniqueness result; application to factorization

The relation between this theorem and the mean-field limit presented in the introduction is as follows. Let Ψ be a solution of the Cauchy problem

$$i\partial_t\Psi(t,x) = -\frac{1}{2}\Delta_x\Psi(t,x) + \left(\int V\big(|x-y|\big)\big|\Psi(t,y)\big|^2\,\mathrm{d}y\right)\Psi(t,x), \quad \Psi(0,x) = \Psi^{\text{in}}(x), \quad x \in \mathbf{R}^3, \tag{13}$$

with $\Psi^{\text{in}} \in \mathrm{H}^1(\mathbf{R}^3)$ such that

$$\int \big|\Psi^{\text{in}}(x)\big|^2\,\mathrm{d}x = 1, \qquad \iint V\big(|x-y|\big)\big|\Psi^{\text{in}}(x)\Psi^{\text{in}}(y)\big|^2\,\mathrm{d}x\,\mathrm{d}y < \infty. \tag{14}$$

(*See* [6] for the existence and uniqueness theory for the mean-field Schrödinger equation.) One can check by inspection that the factorized initial data

$$\Psi_N^{\text{in}}(X_N) = \prod_{k=1}^N \Psi^{\text{in}}(x_k) \tag{15}$$

satisfies the conditions of Theorem 2.1 and that

$$\rho_n(t, X_n, Y_n) = \prod_{k=1}^n \Psi(t, x_k)\overline{\Psi(t, y_k)} \tag{16}$$

is a solution of the inifinite hierarchy (10). If it was known that (10) with initial data deduced from (16) and (15) has a unique solution, Theorem 2.1 would imply that the whole sequence of n-marginals $\rho_{N,n}$ associated to the solution of the N-body Schrödinger equation (6) converges as $N \to +\infty$ to the factorized n-body density matrix (16) in $\mathrm{L}^\infty(\mathbf{R}_+; \mathcal{L}^1(\mathrm{L}^2(\mathbf{R}^{3n})))$ weak-*, built on the solution of the mean-field Schödinger equation (13).

This can be handled by the following abstract uniqueness result. Let E_n be a sequence of Banach spaces indexed by $n \in \mathbf{N}^*$ with norm denoted by $\|\cdot\|_n$. Let A_n be the generator of a strongly continuous group of isometries $U_n(t)$ in E_n and $L_{n,n+1}$ be a bounded linear operator from E_{n+1} to E_n. Consider, for each $n \geqslant 1$, the Cauchy problem

$$u_n'(t) = U_n(-t)L_{n,n+1}U_{n+1}(t)u_{n+1}(t), \quad u_n(0) = 0. \tag{17}$$

The next result is a abstract variant of corollary 5.1 in [1].

THEOREM 3.1. – *Assume that the family of operators $L_{n,n+1}$ satisfies the bound*

$$\|L_{n,n+1}\|_{\mathcal{L}(E_{n+1},E_n)} \leqslant Cn, \quad n \geqslant 1, \tag{18}$$

for some $C > 0$. Let $t^* > 0$ and $u_n \in \mathrm{C}^1([0,t^*], E_n)$ for $n \geqslant 1$ be a solution to (17) *satisfying the growth condition*

$$\text{there exists } R > 0 \text{ such that } \sup_{t\in[0,t^*]}\big\|u_n(t)\big\|_n \leqslant R^n. \tag{19}$$

Then $u_n = 0$ on $[0,t^*]$ for all $n \geqslant 1$.

Proof. – For all $r > 0$ define the Banach space

$$B_r = \left\{ v = (v_n)_{n\geqslant 1} \in \prod_{n\geqslant 1} E_n \;\middle|\; \|v\|_r = \sum_{n\geqslant 1} r^n \|v_n\|_n < +\infty \right\},$$

and set $F(v,t) = (U_n(-t)L_{n,n+1}U_{n+1}(t)v_{n+1})_{n\geqslant 1}$. The assumptions on A_n and $L_{n,n+1}$ imply that, for all $r > 0$ and all $v \in B_r$

$$\big\|F(v,t)\big\|_{r_1} \leqslant C \sum_{n\geqslant 1} n r_1^n \big\|v_{n+1}\big\|_{n+1} \leqslant \frac{C}{r-r_1} \sum_{n\geqslant 1} \big(r^n - r_1^n\big) \|v_{n+1}\|_{n+1} \leqslant \frac{C\|v\|_r}{r-r_1}$$

for all $t \in \mathbf{R}$ and all $r_1 \in [0, r[$, by an easy convexity argument. The conclusion follows from the abstract Cauchy–Kowalewski theorem of Nirenberg and Nishida (*see* [9]). □

We seek to apply Theorem 3.1 to the infinite Schrödinger hierarchy (10) by setting

$$(A_n\rho_n)(X_n, Y_n) = \frac{i}{2}(\Delta_{X_n} - \Delta_{Y_n})\rho_n(X_n, Y_n) \quad \text{and} \quad L_{n,n+1} = -i\,\mathcal{C}_{n,n+1}. \tag{20}$$

If the potential V is bounded, one can take $E_n = \mathcal{L}^1(\mathrm{L}^2(\mathbf{R}^{3n}))$; $U_n(t)$ acts on ρ_n by conjugating it with $\mathrm{e}^{it\Delta_{X_n}/2}$ which is a unitary group in $\mathrm{L}^2(\mathbf{R}^{3n})$; therefore it is isometric in E_n. On the other hand a straightforward estimate shows that for all $n \geqslant 1$,

$$\|\mathcal{C}_{n,n+1}\|_{\mathcal{L}(E_{n+1},E_n)} \leqslant 2n\|V\|_{\mathrm{L}^\infty}. \tag{21}$$

Hence Theorem 3.1 applies and together with Theorem 2.1 gives a new proof of the weak coupling limit of the N-body Schrödinger announced by Spohn [10] (who already used the trace norm in however a slightly different way). See Section 5 of [1] for details and for a stability result somewhat analogous to Theorem 3.1.

4. The case of the Coulomb potential

Theorem 2.1 applies to the case of the repulsive Coulomb potential $V(r) = 1/r$. In order to apply Theorem 3.1, one needs to choose the Banach spaces E_n so that (18), and in particular a certain analogue of (21) hold. The Coulomb singularity can be controlled by the inequality

$$\operatorname{trace}|V\rho| \leqslant C \operatorname{trace}\big[(I-\Delta)^{1/2}\rho(I-\Delta)^{1/2}\big], \quad \rho \in \mathcal{L}^1\big(\mathrm{L}^2\big(\mathbf{R}^3\big)\big) \tag{22}$$

which is consequence of the Hardy inequality $\frac{1}{4}|x|^{-2} \leqslant -\Delta$ in $d = 3$ (*see* [8], pp. 203–204). We recall, however, that $A \leqslant B$ does not imply that $\operatorname{trace}|AC| \leqslant \operatorname{trace}|BC|$ even for positive operators. The proof of (22) uses $\operatorname{trace}\sqrt{A^*B^*BA} = \operatorname{trace}\sqrt{BAA^*B^*}$, and that the square root is monotonic for operators.

This leads to the definition of the following norm. Let $S_n = (I - \Delta_{x_n})^{1/2}$ and set $G_n = \prod_{k=1}^n S_k$ for all $n \geqslant 1$. For $T \in \mathcal{L}(\mathrm{L}^2(\mathbf{R}^{3n}))$, define $\|T\|_n = \operatorname{trace}(|G_nTG_n|)$ and consider the Banach space

$$E_n := \big\{T \in \mathcal{L}\big(\mathrm{L}^2\big(\mathbf{R}^{3n}\big)\big) \mid \|T\|_n < +\infty\big\}. \tag{23}$$

Because $\mathrm{e}^{it\Delta_{X_n}/2}$ commutes with G_n, the operator A_n defined in (20) generates a strongly continuous group of isometries on E_n. With this norm, one can prove that (18) holds.

Our next task is to verify (19) for the limiting density matrices. Denote $\mathcal{H}_N^0 := -\sum_{j=1}^N \Delta_{x_j}$. For pure states (3) satisfying the symmetry condition (4), the norm in E_n (23) for n fixed is uniformly bounded by the norm $|||\Psi_N|||_{N,n} = \langle\Psi_N, (\frac{1}{N}\mathcal{H}_N^0)^n\Psi_N\rangle^{1/2} + \|\Psi_N\|_{\mathrm{L}^2}$. Since $(\mathcal{H}_N)^n$ is conserved by the flow of (6), to control $(\mathcal{H}_N^0)^n$ it would suffice to establish that

$$C^{-n}(\mathcal{H}_N)^n \leqslant \big(\mathcal{H}_N^0\big)^n \leqslant C^n(\mathcal{H}_N)^n, \tag{24}$$

and that for the initial data we have $|||\Psi_{N|t=0}|||_{N,n} \leqslant R^n$.

The bound (24) as it stands is incorrect due to the Coulomb potential. In the expression $\mathcal{H}_N^n$ the Coulomb singularity is taken to high powers and the resulting singularities cannot be controlled by higher derivatives.

Therefore, we need to cutoff the Coulomb singularity in the Hamiltonian $\mathcal{H}_N$ and estimate the error. Similarly the bound $|||\Psi_{N|t=0}|||_{N,n} \leqslant R^n$ requires the initial data to be essentially C^∞, which is a very serious restriction. This restriction can be removed by smoothing an H^2 initial data and comparing the solutions of N-body Schrödinger equation with the original initial data and the smoothed one. Both the cutoff and the smoothing length scales depend on N.

These estimates also imply the analogue of theorem 2.1 in the weak-* topology of $\prod_{n\geqslant 1} L^\infty(\mathbf{R}_+; E_n)$ for the smoothed initial data and for the Hamiltonian with a cutoff. However, the cutoff estimates can be controlled only in a weaker space. This leads to the the following derivation of the Schrödinger–Poisson equation. See [3] for the proof.

THEOREM 4.1. – *Let $V(r) = \pm 1/r$ be the attractive or repulsive Coulomb potential. Let $\Psi^{\mathrm{in}} \in H^2(\mathbf{R}^3)$ satisfy $\|\Psi^{\mathrm{in}}\|_{L^2} = 1$, and let Ψ be the solution of the Schrödinger–Poisson equation* (13). *Let Ψ_N be the solution of the N-body Schrödinger equation* (6). *Let $\rho_{N,n}$ be, for all $n \geqslant 1$, the n-marginal of the density matrix* (3) *of Ψ_N defined as in* (7). *As $N \to \infty$, $\rho_{N,n}$ converges in $L^\infty_{\mathrm{loc}}(\mathbf{R}_+; \mathcal{L}^1(L^2(\mathbf{R}^{3n})))$ weak-* to the factorized solution*

$$\rho_n(t, X_n, Y_n) = \prod_{k=1}^{n} \Psi(t, x_k)\overline{\Psi(t, y_k)}.$$

Although the uniqueness of the solution to the hierarchy (10) can always be established if we impose a very strong norm on the density matrices, such a result is useful only if we can prove that the limiting density matrices are bounded in that norm. There are very few a priori estimates which can be proved for solutions of many-body Schrödinger equations. The conservation of the L^2 norm and the energy has been widely used in the literature. Clearly, the higher powers of the energy are also conserved, but we are not aware of their application prior to this work. The key point in [3] is that this high power of the energy, together with a proper cutoff procedure for the Coulomb singularity and a regularization of the initial data, provides the basic a priori estimates needed for the uniqueness of the hierarchy.

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