Atomism and Quantization

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Abstract

Within the framework of the theory of interacting classical and quantum gases it is shown that the atomistic constitution of gases can be understood as a consequence of (second) quantization of a continuum theory of gases. In this note this is explained in some detail for the theory of non-relativistic interacting Bose gases, which can be viewed as the second quantization of a continuum theory whose dynamics is given by the Hartree equation.
Conversely, the Hartree equation emerges from the theory of Bose gases in the mean-field limit. It is shown that, for such systems, the time evolution of "observables" commutes with their Wick quantization, up to quantum corrections that tend to 0 in the mean-field limit. This is a Egorov-type theorem.

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1 Introduction

Physics in the 20$^{\text{th}}$ Century has been marked by the experimental verification and theoretical vindication of one basic paradigm and three revolutions. The paradigm is *Atomism*; it assumes that matter is composed of atoms. It was created by ancient Greek natural philosophers. Newton, Maxwell, Boltzmann and others were ardent advocates of an atomistic view of matter. In his treatise "Opticks", Newton writes: "All things being considered, it seems probable to me that God in the Beginning formed Matter in solid, massy, hard, impenetrable, moveable Particles ...." Light was included in Newton's atomistic views of Nature: He held the opinion that light consisted of pointlike particles.

The three revolutions alluded to above are:

(1) The passage from *classical* to *quantum mechanics*.

(2) The replacement of Newton's absolute space and time by the space-time continuum of the *special theory of relativity*, i.e., Minkowski space, and of Galilei covariance by Poincaré covariance.

(3) The passage from a rigid space-time to the "dynamical" space-time of the *general theory of relativity* that depends on the distribution of matter and describes the gravitational interactions of matter.

Traces of Atomism and of the three revolutions just described miraculously appear in two Laws of Nature:

(i) Newton's Law of Universal Gravitation

$$\mathbf{F}(\mathbf{r}) \;=\; -\frac{Gm_1m_2}{r^3}\mathbf{r}\,, \tag{1}$$

where G is Newton's gravitational constant, and

(ii) Planck's Law for the spectral energy density of black body radiation

$$\rho(T,\nu) \;=\; 2\frac{4\pi\nu^2}{c^3}\frac{h\nu}{e^{h\nu/kT}-1}\,, \tag{2}$$

where c denotes the speed of light, h is Planck's constant, and k is Boltzmann's constant.

Planck recognized that these two laws contain four dimensionful fundamental constants of Nature, k, h, c, and $l_P := \sqrt{Ghc^{-3}}$ (the "Planck length"), which (together with the universal gas constant R or Faraday's constant F) appear to determine all other fundamental constants. He foresaw that every one of these four constants would stand for a revolution in the world view of Physics: k and h stand for Atomism and Quantum Theory, which are fellow travelers, c for special relativity, and c and l_P for general relativity.

Neither Atomism nor the three revolutions which occured during the first quarter of the 20$^{\text{th}}$ Century were immediately widely accepted by the physicists. Before 1900, Planck rejected Atomism. Surprisingly, the chemist Ostwald was an outspoken adversary of the atomistic view, and Mach wrote, as late as 1913: "I must [...] assuredly disclaim to be a forerunner of the relativists as I withhold from the *atomistic belief* of the present day." Einstein's atomistic view of electromagnetism, in particular his concept of light quanta or photons, encountered disbelief and doubt until the 1920's. For further historical details, see [18].

Einstein's discovery of photons has the interesting feature that it links the atomistic constitution of light to *quantization*: Starting from the Wien-Planck "quantum theory" of black body radiation, he derives a formula for the entropy difference of black-body radiation of frequency ν in an energy interval ΔE inside two containers of volumes V and V_0, respectively:

$$S - S_0 \;=\; k \log \left(\frac{V}{V_0} \right)^{\Delta E / h\nu} . \tag{3}$$

Comparing this expression with Boltzmann's principle, $S = k \log W$, where W is the probability of the state of a system, he deduces that

$$W \;=\; W_0 \left(\frac{V}{V_0} \right)^{\Delta E / h\nu} . \tag{4}$$

Comparing this formula with a corresponding formula for the relative probability of the states of an ideal gas of N independent particles in containers of volumes V and V_0, respectively, namely $W = W_0 (V/V_0)^N$, he concludes that "monochromatic radiation of low density behaves, in relation to the theory of heat, as if it were composed of independent energy quanta of magnitude $h\nu$;" (with $N = \Delta E / h\nu$ the number of quanta).

Apparently, the atomistic constitution of light emerges from the *quantization* of Maxwell's theory of the electromagnetic field. In this note, we discuss another example of the same phenomenon that the atomistic constitution of matter can be viewed as a consequence of "quantization": a gas of interacting bosonic atoms. The quantum theory of this system turns out to be the "*second quantization*" of a continuum field theory of interacting gases that can be viewed as a classical Hamiltonian system with infinitely many degrees of freedom – just like Maxwell's theory.

The observation that Atomism can be seen as a consequence of quantization helps to complete a picture first suggested by the late Moshe Flato, namely that the new physical theories born in the three revolutions mentioned above can all be understood as arising from "deformations" of precursor theories. We pause to sketch what may be meant by this claim.

Physical systems Σ can be characterized by the following data:

(a) An associative $*$-algebra $\mathcal{A}_\Sigma$, parametrizing the possible outcomes of experiments on Σ (the "*kinematical algebra*" of Σ);

(b) a convex set $\mathscr{S}_\Sigma$ of states of Σ, usually defined as positive linear functionals on $\mathcal{A}_\Sigma$;

(c) the *symmetries* $\mathcal{G}_\Sigma$ of Σ, most often described in terms of $*$-automorphisms (or $*$-endomorphisms) of $\mathcal{A}_\Sigma$.

Given a class of structurally identical systems, one also wishes to specify

(d) an operation $\vee$, acting on pairs of data $\big((\mathcal{A}_{\Sigma_1}, \mathscr{S}_{\Sigma_1}, \mathcal{G}_{\Sigma_1}), (\mathcal{A}_{\Sigma_2}, \mathscr{S}_{\Sigma_2}, \mathcal{G}_{\Sigma_2})\big)$ characterizing two physical systems, Σ_1 and Σ_2, that associates with Σ_1 and Σ_2 a *composed system* $\Sigma_1 \vee \Sigma_2$, characterized by $(\mathcal{A}_{\Sigma_1 \vee \Sigma_2}, \mathscr{S}_{\Sigma_1 \vee \Sigma_2}, \mathcal{G}_{\Sigma_1 \vee \Sigma_2})$.

Prominent examples of physical systems are *Hamiltonian systems*. For a Hamiltonian system Σ, $\mathcal{A}_\Sigma$ is the abelian algebra of smooth functions on a symplectic manifold Γ_Σ, the phase space of Σ. The Poisson bracket equips $\mathcal{A}_\Sigma$ with the structure of a Lie algebra. The space $\mathscr{S}_\Sigma$ of states of Σ is given by the probability measures on Γ_Σ; pure states correspond to Dirac δ-functions localized in points of Γ_Σ. The symmetries of Σ are described by (some subgroup of) symplectomorphisms of Γ_Σ. Two systems Σ_1 and Σ_2 are composed to a system $\Sigma_1 \vee \Sigma_2$ by taking the Cartesian product, $\Gamma_{\Sigma_1} \times \Gamma_{\Sigma_2} =: \Gamma_{\Sigma_1 \vee \Sigma_2}$, of their phase spaces, etc.

A system Σ characterized by $(\mathcal{A}_\Sigma, \mathscr{S}_\Sigma, \mathcal{G}_\Sigma)$ can be "deformed" to a new system $\widehat{\Sigma}$ by deforming its kinematical algebra $\mathcal{A}_\Sigma$ to a new *associative* $*$*-algebra* $\mathcal{A}_{\widehat{\Sigma}}$, and, correspondingly, deforming $\mathscr{S}_\Sigma$ to a new convex set of states $\mathscr{S}_{\widehat{\Sigma}}$; and/or by deforming the symmetries $\mathcal{G}_\Sigma$ to a new set of symmetries $\mathcal{G}_{\widehat{\Sigma}}$. In addition, a class of structurally identical deformed systems may admit a new operation of composition $\vee$.

From this point of view, *quantization* of a classical Hamiltonian system Σ consists of deforming $\mathcal{A}_\Sigma = C^\infty(\Gamma_\Sigma)$ to a new associative, but usually non-abelian $*$-algebra $\mathcal{A}_{\widehat{\Sigma}}$, replacing the Poisson bracket by $\frac{i}{\hbar} \times$ (commutator of elements in $\mathcal{A}_{\widehat{\Sigma}}$), and, correspondingly, passing from $\mathscr{S}_\Sigma$ to the set $\mathscr{S}_{\widehat{\Sigma}}$ of positive linear functionals on $\mathcal{A}_{\widehat{\Sigma}}$, and replacing $\mathcal{G}_\Sigma$ by a group $\mathcal{G}_{\widehat{\Sigma}}$ of $*$-automorphisms of $\mathcal{A}_{\widehat{\Sigma}}$. The parameter $\hbar$ (Planck's constant) plays the role of the "*deformation parameter*". In the sense of formal power series, the quantization of Hamiltonian systems is always possible; see [2, 6, 13].

If the symmetries $\mathcal{G}_\Sigma$ of a physical system Σ are described in terms of representations of a *Lie group* G as $*$-automorphisms of $\mathcal{A}_\Sigma$, the symmetries $\mathcal{G}_{\widehat{\Sigma}}$ of a deformation $\widehat{\Sigma}$ of Σ might arise from a deformation of the symmetry group G to a new symmetry group $\widehat{G}$. For example, if G is the Galilei group then $\widehat{G}$ may be the Poincaré group. In this well known example, the deformation parameter is c^{-1} (the inverse of the speed of light). Another example is encountered if one replaces the symmetry group of translations of a charged particle confined to a plane $\mathbb{R}^2$ by the non-commutative Heisenberg group of magnetic translations, which is a central extension of the group $\mathbb{R}^2$ with deformation parameter ("central charge") given by qBc^{-1}, where q is the charge of the particle and B is the component of the external magnetic field perpendicular to the plane of the system.

If $\widehat{\Sigma}_1$ and $\widehat{\Sigma}_2$ are quantizations of classical Hamiltonian systems Σ_1 and Σ_2, then composition $\vee$ is defined in terms of the tensor product

$$\mathcal{A}_{\widehat{\Sigma}_1 \vee \widehat{\Sigma}_1} \;:=\; \mathcal{A}_{\widehat{\Sigma}_1} \otimes \mathcal{A}_{\widehat{\Sigma}_2} \,. \tag{5}$$

If $\Sigma_1, \ldots, \Sigma_n$ are *identical* systems, $\Sigma_j \simeq \Sigma$ for $j = 1, \ldots, n$, then

$$\mathcal{A}_{\widehat{\Sigma}_1 \vee \cdots \vee \widehat{\Sigma}_n} \;=\; \mathcal{A}_{\widehat{\Sigma}_1} \otimes_s \cdots \otimes_s \mathcal{A}_{\widehat{\Sigma}_n} \,, \tag{6}$$

where $\otimes_s$ denotes the *symmetric* tensor product. If one studies the composition of the *Hilbert spaces of state vectors* (rather than of states) of the systems $\widehat{\Sigma}_1, \ldots, \widehat{\Sigma}_n$, one is led to consider representations of the permutation group of n elements or of the braid group on n strands describing the transformations of state vectors under exchange of identical subsystems. These representations describe what is commonly called the "(quantum) *statistics*" of $\widehat{\Sigma}$ (Bose-, Fermi-, or fractional statistics). See [3, 7] for a general analysis.

A quantum system $\widehat{\Sigma}$ with fractional statistics, i.e., whose quantum statistics is described by representations of the braid groups, may have symmetries $\mathcal{G}_{\widehat{\Sigma}}$ described in terms of representations of some "quantum group". Many examples of quantum groups arise as associative deformations of the universal enveloping algebra of a Lie algebra with the structure of a quasi-triangular Hopf algebra.

The common theme in this discussion is the "deformation theory of algebras" [9], namely of associative algebras, Hopf algebras, group algebras, Lie algebras, etc. Quantum mechanics arises from a deformation of associative algebras, the kinematical algebras, and the associated deformation of states; special relativity from a deformation of space-time and the associated Lie algebra of space-time symmetries. Certain forms of fractional statistics can be understood as arising from deformations of the rule for the composition of identical systems.

In this note we are interested in understanding *atomistic theories of matter as "(second) quantizations" of continuum theories of matter*, the deformation theory involved being the one of associative $*$-algebras. Although this point of view has been around, at least implicitly, for a long time, it has rarely been emphasized explicitly. As mentioned above, it underlies Einstein's theory of photons. More generally, any quantum field theory that is the quantization of a classical Hamiltonian field theory provides an example of this point of view. In this note, we illustrate it in terms of the theory of interacting (classical and quantum) gases. We focus on the discussion of quantum gases. A more complete discussion that also includes classical gases and fluids will appear elsewhere.

A glimpse of the idea that Quantum Theory and Atomism may be inseparable companions may be gained by studying the classical statistical mechanics of identical particles: The Liouville measure on the phase space of such systems has the dimension $(\text{action})^f$, where f is the number of degrees of freedom. In order to define the partition functions of such systems as dimensionless quantities, one must divide the Liouville measure by the f^{th} power of a constant (h) with the dimension of an action. Moreover, in order for the basic thermodynamic potentials to be extensive, one must consider identical particles to be *indistinguishable* and divide the partition functions by $N!$, where N is the number of particles – as first recognized by Gibbs.

For the purposes of this note, a *classical gas* is described as a *continuous medium*, whose states are given by specifying a *mass density*, $d\mu(x,p) = Mf(x,p)\,dx\,dp$, on the Cartesian product of physical space $\mathbb{R}^3$ and momentum space $\mathbb{R}^3$, where M has the dimension of a mass; $Mf(x,p)\,dx\,dp$ is the mass of the gas in the cell $dx\,dp$ around the point $(x,p) \in \mathbb{R}^3 \times \mathbb{R}^3$. The total mass of the gas is $\int d\mu(x,p) = \nu M$, where $\nu := \int dx\,dp\,f(x,p)$ is a dimensionless constant. Apparently,

$$\rho(x) \;:=\; \int dp\, M f(x,p) \tag{7}$$

is the mass density at the point x in space. An example of an equation of motion for $f(x,p)$ is the *Vlasov equation*

$$\partial_t f_t(x,p) \;=\; -\frac{N}{M}(p\cdot\nabla_x f_t)(x,p) + (\nabla V_{\text{eff}}[f_t]\cdot\nabla_p f_t)(x,p)\,, \tag{8}$$

where N is a dimensionless quantity, t denotes time, and

$$V_{\text{eff}}[f](x) \;:=\; V(x) + \int dy\,\phi(x-y)\int dp\, f(y,p)\,. \tag{9}$$

Here V is the potential of external forces acting on the gas and ϕ a two-body potential describing self-interactions of the gas.

The Vlasov equation arises as the mean-field limit of a classical Hamiltonian system of $n = \nu N$ point particles of mass $m = M/N$, with trajectories $(x_j(t))_{j=1}^n$, moving in an external potential V and interacting through two-body forces with potential $\frac{1}{N}\phi(x_i - x_j)$, $1 \le i < j \le n$. Then $f_t(x,p)$ is given by

$$f_t(x,p) \;=\; \underset{n\to\infty}{\text{w*-lim}}\, \frac{\nu}{n} \sum_{j=1}^{n} \delta(x - x_j(t))\, \delta(p - m\dot{x}_j(t))\,, \tag{10}$$

for all times t, provided that (10) holds for $t = 0$; see [1, 17].

It is of some interest to note that the Vlasov dynamics may be interpreted as a Hamiltonian dynamics on an infinite-dimensional affine phase space, $\Gamma_{\text{cl.}}$. (For related, but somewhat different observations, see [14, 15]). To see this, we write

$$f(x,p) \;=\; \overline{\alpha(x,p)}\alpha(x,p)\,, \tag{11}$$

where $\big(\overline{\alpha(x,p)}, \alpha(x,p)\big)$ are complex coordinates of $\Gamma_{\text{cl.}}$. In particular, $\|\alpha\|_2^2 = \nu$. We choose $\Gamma_{\text{cl.}}$ to be a weighted Sobolev space of index 1 and equip it with the Poisson brackets

$$\{\alpha(x,p), \alpha(y,q)\} \;=\; \{\overline{\alpha(x,p)}, \overline{\alpha(y,q)}\} \;=\; 0\,, \tag{12a}$$

$$\{\alpha(x,p), \overline{\alpha(y,q)}\} \;=\; i\delta(x-y)\,\delta(p-q)\,. \tag{12b}$$

A Hamilton functional $\mathscr{H}_{\text{Vl.}}$ is defined on $\Gamma_{\text{cl.}}$ by

$$\begin{aligned}\mathscr{H}_{\text{Vl.}}(\overline{\alpha},\alpha) \;:=\; & i\int dx\, dp\, \overline{\alpha(x,p)}\Big[-\frac{N}{M}p\cdot\nabla_x + \nabla V(x)\cdot\nabla_p\Big]\alpha(x,p) \\ & + i\int dx\, dp\, \overline{\alpha(x,p)}\Big[\int dy\, dq\, \nabla\phi(x-y)\, |\alpha(y,q)|^2\Big]\cdot\nabla_p\alpha(x,p)\,. \end{aligned} \tag{13}$$

The Hamiltonian equations of motion for α,

$$\dot{\alpha}_t(x,p) \;=\; \{\mathscr{H}_{\text{Vl.}}, \alpha_t(x,p)\}\,, \tag{14}$$

and for $\overline{\alpha}$ then imply the Vlasov equation for $f = \overline{\alpha}\alpha$. This formulation of the Vlasov dynamics can serve as a starting point to recover the *atomistic Hamiltonian mechanics of point particles* by "deformation quantization", i.e., by replacing the Poisson brackets (12) by $iN \times$ [commutator of annihilation and creation operators], as will be shown elsewhere. Here we pass to a "first-quantized" version of the Vlasov equation: the *Hartree equation* (see Section 3).

We replace (11) by the formula

$$f_\hbar(x,p) \;:=\; \frac{1}{(2\pi)^3}\int dy\, e^{-iy\cdot p}\, \overline{\psi\Big(x - \frac{\hbar y}{2}\Big)}\psi\Big(x + \frac{\hbar y}{2}\Big)\,, \tag{15}$$

i.e., $f_\hbar$ is given as the *Wigner transform* of a wave function $\psi \in L^2(\mathbb{R}^3)$, with $\|\psi\|_2^2 = \nu$. The dynamics of ψ is given by the Hartree equation

$$i\hbar\partial_t\psi_t(x) \;=\; \Big[-\frac{\hbar^2}{2m}\Delta + V(x)\Big]\psi_t(x) + \Big[\int dy\, |\psi_t(y)|^2\phi(x-y)\Big]\psi_t(x)\,, \tag{16}$$

where $m = M/N$ (= mass of a particle). It is shown in [11, 16] that if $f_{\hbar,t}$ is defined as the Wigner transform (15) of $\psi_{\hbar,t}$, where $\psi_{\hbar,t}$ is a solution of (16) with initial data $\psi_{\hbar,0}$ satisfying $\|\psi_{\hbar,0}\|_2^2 = \nu$, then $\lim_{\hbar\searrow 0} f_{\hbar,t}$ solves the Vlasov equation (8) with initial data

$\lim_{\hbar \searrow 0} f_{\hbar,0}$. Equation (16) can be viewed as the field equation of a classical Hamiltonian field theory for the wave field ψ. To see this, we define an affine phase space $\Gamma = \Gamma_{\mathrm{qu.}}$ to be given by a complex weighted Sobolev space of index 1 equipped with Poisson brackets

$$\{\psi(x), \psi(y)\} \;=\; \{\overline{\psi}(x), \overline{\psi}(y)\} \;=\; 0\,, \tag{17a}$$

$$\{\psi(x), \overline{\psi}(y)\} \;=\; i\,\delta(x-y)\,. \tag{17b}$$

We define a Hamilton functional $\mathscr{H}_{\mathrm{Ht.}}$ on Γ by

$$\mathscr{H}_{\mathrm{Ht.}}(\overline{\psi}, \psi) \;:=\; \frac{1}{\hbar} \int dx\, \overline{\psi}(x) \Big[-\frac{\hbar^2}{2m}\Delta + V(x) \Big] \psi(x) + \frac{1}{2\hbar} \int dx \int dy\, |\psi(x)|^2\, \phi(x-y)\, |\psi(y)|^2\,. \tag{18}$$

Then the Hamiltonian equations of motion for ψ,

$$\dot{\psi}_t(x) \;=\; \{\mathscr{H}_{\mathrm{Ht.}}, \psi_t(x)\}\,, \tag{19}$$

reproduce the Hartree equation (16).

In this note we show that if the Poisson brackets (17) are replaced by the *commutators*

$$[\widehat{\psi}_N(x), \widehat{\psi}_N(y)] \;=\; [\widehat{\psi}^*_N(x), \widehat{\psi}^*_N(y)] \;=\; 0\,, \tag{20a}$$

$$[\widehat{\psi}_N(x), \widehat{\psi}^*_N(y)] \;=\; \frac{1}{N}\,\delta(x-y)\,, \tag{20b}$$

we obtain the *atomistic* quantum mechanics of a non-relativistic, interacting Bose gas, described in the formalism of second quantization, as a *deformation* of the classical Hartree field theory, with deformation parameter $1/N$ (see Section 4). We also show how the Hartree field theory can be recovered from the quantum mechanics of the Bose gas in the *mean-field limit*, where the number n of bosons is proportional to N, with $N \to \infty$. For this purpose, we state a *Egorov-type theorem*, which appears to be a new result, and sketch its proof (Section 5); but see [4, 5, 10, 12, 20] for earlier results. Our considerations can be summarized in the diagram

$$\begin{tikzcd}[column sep=large, row sep=large]
\boxed{\text{QM many-body theory}} \arrow[r, shift right, "\hbar"'] \arrow[d, shift right, "\frac{1}{N}"'] & \boxed{\begin{array}{c}\text{Classical mechanics}\\ \text{of point particles}\end{array}} \arrow[l, shift right] \arrow[d, shift right] \\
\boxed{\text{Hartree dynamics}} \arrow[r, shift right] \arrow[u, shift right] & \boxed{\text{Vlasov dynamics}} \arrow[l, shift right] \arrow[u, shift right]
\end{tikzcd}$$

An arrow $\rightarrow$ stands for the limit $\hbar \searrow 0$, $\leftarrow$ stands for quantization with deformation parameter $\hbar$, $\downarrow$ stands for the mean-field limit ($N \to \infty$), and $\uparrow$ stands for "second quantization" with deformation parameter $1/N$. The diagram is commutative. See [8, 19] for details of related results.

To speculate a little, we propose the idea that classical general relativity emerges from a fundamental quantum theory of gravitation in some kind of classical *and* mean-field limit ($\alpha' \to 0$, $g_s \to 0$, in the jargon of string theory), somewhat similarly to how the Vlasov equation emerges from the quantum theory of interacting Bose gases in the limit $\hbar \to 0$, $N \to \infty$. In this analogy, $\alpha' \sim \hbar$, $g_s \sim 1/N$. (In both examples, double expansions in the two different parameters yield strongly divergent series.) In subsequent sections we explain the left part of the diagram shown above. More general results, in particular ones concerning the entire diagram, and extensions of our results to Fermi gases will be reported elsewhere.

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2 Quantum Bose Gases

We consider a system of n bosons with Hilbert space given by

$$\mathcal{H}^{(n)} \;:=\; L^2_{\mathrm{s}}(\mathbb{R}^{3n}) \;=\; L^2(\mathbb{R}^3)^{\otimes_{\mathrm{s}} n} \tag{21}$$

and Hamiltonian

$$H_N^{(n)} \;=\; H_0^{(n)} + V_N^{(n)}\,, \tag{22}$$

where[2]

$$H_0^{(n)} \;:=\; \sum_{j=1}^{n}\left[-\frac{1}{2m}\Delta_j + V(x_j)\right], \qquad V_N^{(n)} \;:=\; \frac{1}{N}\sum_{1\le i<j\le n}\phi(x_i - x_j)\,. \tag{23}$$

Here the external potential $V \geq 0$ is smooth and polynomially bounded, the interaction potential ϕ is bounded, $m > 0$ is the mass of a particle, and $1/N$ is a dimensionless coupling constant. The dynamics of the system is described by the Schrödinger equation

$$i\partial_t \varphi_t^{(n)} \;=\; H_N^{(n)}\varphi_t^{(n)}\,, \qquad \varphi_t^{(n)} \in \mathcal{H}^{(n)}\,. \tag{24}$$

The mean-field limit is the limit where $n, N \to \infty$ in such a way that $n/N = O(1)$. The physical meaning of this limit is most transparent if the system is described in the formalism of second quantization. Fock space is the Hilbert space given by

$$\mathcal{F} \;:=\; \bigoplus_{n=0}^{\infty}\mathcal{H}^{(n)}\,. \tag{25}$$

Subspaces $\mathcal{F}^{\leq k}$ of finite particle number are defined by

$$\mathcal{F}^{\leq k} \;:=\; \bigoplus_{n=0}^{k}\mathcal{H}^{(n)}\,. \tag{26}$$

Fock space $\mathcal{F}$ carries a representation of the canonical commutation relations (CCR):

$$[\widehat{\psi}_N(x), \widehat{\psi}_N(y)] \;=\; [\widehat{\psi}_N^*(x), \widehat{\psi}_N^*(y)] \;=\; 0\,, \tag{27a}$$

$$[\widehat{\psi}_N(x), \widehat{\psi}_N^*(y)] \;=\; \frac{1}{N}\,\delta(x-y)\,, \tag{27b}$$

[2] Here, and in the following, we work in units such that $\hbar = 1$.

with $\widehat{\psi}_N(x)\Omega = 0$, for all $x, y \in \mathbb{R}^3$, where $\Omega = (1, 0, 0, \dots) \in \mathcal{F}$ is the vacuum. Note that the creation and annihilation operators, $\widehat{\psi}^*_N(x)$, $\widehat{\psi}_N(x)$, are rescaled by a factor of $N^{-1/2}$ as compared to the usual ones. This accounts for the factor $1/N$ in the CCR, in analogy to the usual $\hbar$. Thus $1/N$ is given the role of a deformation parameter. The direct sum of the Hamiltonians (22), acting on Fock space and rescaled by $1/N$, can now be written in terms of the creation and annihilation operators,

$$\widehat{\mathscr{H}_N} \;:=\; \frac{1}{N}\bigoplus_{n=0}^{\infty} H_N^{(n)} \;=\; \widehat{\mathscr{H}_{0,N}} + \widehat{\mathscr{V}_N}\,, \tag{28}$$

where

$$\widehat{\mathscr{H}_{0,N}} \;:=\; \int \widehat{\psi}^*_N(x)\Big[-\frac{1}{2m}\Delta + V(x)\Big]\widehat{\psi}_N(x)\,dx\,, \tag{29}$$

$$\widehat{\mathscr{V}_N} \;:=\; \frac{1}{2}\int dx\int dy\; \widehat{\psi}^*_N(x)\widehat{\psi}^*_N(y)\,\phi(x-y)\,\widehat{\psi}_N(y)\widehat{\psi}_N(x)\,. \tag{30}$$

Thus the Schrödinger equations (24), with $n = 0, 1, 2, \dots$, imply the equation

$$\frac{i}{N}\,\partial_t\Phi_t \;=\; \widehat{\mathscr{H}_N}\Phi_t\,, \qquad \Phi_t \in \mathcal{F}\,. \tag{31}$$

Next, we define a kinematical algebra of operators describing the physical properties of the system. Let $a^{(p)} \in B(\mathcal{H}^{(p)})$ be a bounded operator on the p-particle Hilbert space. Let $a^{(p)}(x_1, \dots, x_p; y_1, \dots y_p)$ be the distribution kernel associated to $a^{(p)}$ by the nuclear theorem. To $a^{(p)}$ we associate an operator $\widehat{A}_N(a^{(p)})$ on Fock space by

$$\widehat{A}_N(a^{(p)}) \;:=\; \iint \prod_{i=1}^{p}\widehat{\psi}^*_N(x_i)\,dx_i\; a^{(p)}(x_1, \dots, x_p; y_1, \dots y_p)\prod_{j=1}^{p}\widehat{\psi}_N(y_j)\,dy_j\,. \tag{32}$$

For bounded $a^{(p)}$, $\widehat{A}_N(a^{(p)})$ is a bounded operator on $\mathcal{F}^{\le k}$, for all $k < \infty$, densely defined on $\mathcal{F}$ and closable. We define a $*$-algebra

$$\widehat{\mathcal{A}} \;:=\; \big\langle \widehat{A}_N(a^{(p)}) \;:\; a^{(p)} \in B(\mathcal{H}^{(p)}),\, p = 0, 1, 2, \dots \big\rangle\,, \tag{33}$$

where $\langle\cdot\rangle$ denotes the linear span. By definition $\widehat{\mathcal{A}}$ is a linear space. It is actually a $*$-algebra of unbounded operators on $\mathcal{F}$. This can be seen from the following properties of the operators $\widehat{A}_N$. Their proof is merely an exercise in Wick ordering.

(i) Let $a^{(p)} \in B(\mathcal{H}^{(p)})$ and $b^{(q)} \in B(\mathcal{H}^{(q)})$. Then

$$\widehat{A}_N(a^{(p)})\,\widehat{A}_N(b^{(q)}) \;=\; \sum_{l=0}^{\min(p,q)}\binom{p}{l}\binom{q}{l}\frac{l!}{N^l}\,\widehat{A}_N(a^{(p)} \underset{l}{\rightharpoonup} b^{(q)})\,, \tag{34}$$

where $a^{(p)} \underset{l}{\rightharpoonup} b^{(q)} := P_{\mathrm{s}}\,(a^{(p)} \otimes \mathbb{1}^{(q-l)})\,(\mathbb{1}^{(p-l)} \otimes b^{(q)})$ is a bounded operator on $\mathcal{H}^{(p+q-l)}$. Here P_{s} is the orthogonal projection onto the subspace of vectors symmetric under the exchange of particles. In terms of operator kernels this reads

$$\begin{aligned}
&(a^{(p)} \underset{l}{\rightharpoonup} b^{(q)})(x_1, \dots x_{p+q-l}; y_1, \dots, y_{p+q-l})\\
&= P_{\mathrm{s}}\int\prod_{i=1}^{l} du_i\; a^{(p)}(x_1, \dots, x_p; y_1, \dots, y_{p-l}, u_1, \dots, u_l)\\
&\qquad\cdot b^{(q)}(u_1, \dots, u_l, x_{p+1}, \dots, x_{p+q-l}; y_{p-l+1}, \dots, y_{p+q-l})\,.
\end{aligned} \tag{35}$$

(ii) An immediate consequence of (i) is

$$\big[\widehat{A}_N(a^{(p)}),\, \widehat{A}_N(b^{(q)})\big] \;=\; \sum_{l=1}^{\min(p,q)} \binom{p}{l}\binom{q}{l} \frac{l!}{N^l}\, \widehat{A}_N\big(\big[a^{(p)} \underset{l}{\rightharpoonup} b^{(q)}\big]\big)\,, \tag{36}$$

where $\big[a^{(p)} \underset{l}{\rightharpoonup} b^{(q)}\big] := a^{(p)} \underset{l}{\rightharpoonup} b^{(q)} - b^{(q)} \underset{l}{\rightharpoonup} a^{(p)}$.

(iii) $\widehat{A}_N(a^{(p)})^* = \widehat{A}_N(a^{(p)*})$, where

$$a^{(p)*}(x_1, \ldots, x_p; y_1, \ldots y_p) \;=\; \overline{a^{(p)}(y_1, \ldots, y_p; x_1, \ldots x_p)}\,. \tag{37}$$

(iv) On the subspaces $\mathcal{F}^{\leq k}$ of bounded particle number, $\widehat{A}_N(a^{(p)})$ is bounded and

$$\Big\| \widehat{A}_N(a^{(p)})\Big|_{\mathcal{F}^{\leq \nu N}} \Big\| \;\leq\; \nu^p\, \|a^{(p)}\|\,. \tag{38}$$

Furthermore, the operators in $\widehat{\mathcal{A}}$ are gauge-invariant: Under the $*$-automorphism τ_θ, given by

$$\tau_\theta(\widehat{\psi}_N(x)) \;:=\; e^{-i\theta}\widehat{\psi}_N(x) \qquad \tau_\theta(\widehat{\psi}^*_N(x)) \;=\; e^{i\theta}\widehat{\psi}^*_N(x)\,, \tag{39}$$

we have $\tau_\theta(\widehat{A}) = \widehat{A}$, for all $\widehat{A} \in \widehat{\mathcal{A}}$. Note that $(\tau_\theta)_{\theta\in\mathbb{R}}$ can be implemented by the one-parameter unitary group $(U(\theta))_{\theta\in\mathbb{R}}$ on $\mathcal{F}$ generated by the number operator

$$\widehat{\mathscr{N}} := N \int dx\; \widehat{\psi}^*_N(x)\widehat{\psi}_N(x)\,. \tag{40}$$

3 A Hamiltonian Continuum Theory of Gases

In this section, we consider a "classical" Hamiltonian system with phase space $\Gamma = H^1_{\mathrm{W}}(\mathbb{R}^3)$, a weighted complex Sobolev space of index 1, defined as the quadratic form domain of the operator $-\frac{\Delta}{2m} + V$. On Γ we use complex coordinates $\psi(x), \overline{\psi}(x)$ and define a Poisson bracket $\{\,\cdot\,,\,\cdot\,\}$ through

$$\{\psi(x), \psi(y)\} \;=\; \{\overline{\psi}(x), \overline{\psi}(y)\} \;=\; 0\,, \tag{41a}$$
$$\{\psi(x), \overline{\psi}(y)\} \;=\; i\,\delta(x-y)\,. \tag{41b}$$

A Hamilton functional is defined by

$$\mathscr{H}(\overline{\psi}, \psi) \;=\; \mathscr{H}_0(\overline{\psi}, \psi) + \mathscr{V}(\overline{\psi}, \psi)\,, \tag{42}$$

where

$$\mathscr{H}_0(\overline{\psi}, \psi) \;:=\; \int dx\; \overline{\psi}(x)\Big[-\frac{1}{2m}\Delta + V(x)\Big]\psi(x) \tag{43}$$

$$\mathscr{V}(\overline{\psi}, \psi) \;:=\; \frac{1}{2}\int dx \int dy\; |\psi(x)|^2\, \phi(x-y)\, |\psi(y)|^2\,. \tag{44}$$

The Hamiltonian equations of motion corresponding to $\mathscr{H}$ are given by the *Hartree equation*

$$\partial_t\psi_t(x) \;=\; \{\mathscr{H}, \psi_t(x)\} \;=\; -i\Big[-\frac{1}{2m}\Delta + V(x)\Big]\psi_t(x) - i\big(\phi * |\psi_t|^2\big)(x)\,\psi_t(x)\,, \tag{45}$$

where $*$ denotes convolution; ($\overline{\psi}_t(x)$ satisfies the complex conjugate equation). Since V is smooth and polynomially bounded and ϕ bounded, (45) has global solutions for arbitrary initial conditions $\psi_0 \in \Gamma$ [3]. This can be used to define a global symplectic flow Φ^t on Γ by

$$\Phi^t(\psi) \;:=\; \psi_t\,, \tag{46}$$

where ψ_t is the solution of (45) with initial data ψ.

The function $\mathscr{N}(\overline{\psi},\psi) := \int dx\, |\psi(x)|^2 = \|\psi\|_2^2$ generates the gauge transformations

$$\psi(x) \mapsto e^{-i\theta}\psi(x)\,, \qquad \overline{\psi}(x) \mapsto e^{i\theta}\overline{\psi}(x)\,. \tag{47}$$

Gauge invariance of $\mathscr{H}$ and Noether's theorem imply that the "charge" $\mathscr{N}$ is a conserved quantity of the flow Φ^t. Since the system is autonomous, the energy $\mathscr{H}$ is conserved as well.

We introduce an algebra $\mathcal{A}$ of "classical" observables in analogy to $\widehat{\mathcal{A}}$ defined above. For $a^{(p)} \in B(\mathcal{H}^{(p)})$ we define the function $A(a^{(p)})$ on Γ by

$$A(a^{(p)})(\overline{\psi},\psi) \;:=\; \iint \prod_{i=1}^{p} \overline{\psi}(x_i)\, dx_i\; a^{(p)}(x_1,\dots,x_p;y_1,\dots y_p) \prod_{j=1}^{p} \psi(y_j)\, dy_j\,, \tag{48}$$

and set

$$\mathcal{A} \;:=\; \big\langle A(a^{(p)}) \;:\; a^{(p)} \in B(\mathcal{H}^{(p)}),\, p=0,1,2,\dots \big\rangle\,. \tag{49}$$

This is clearly an abelian $*$-algebra under pointwise multiplication, and it is equipped with a Poisson bracket. A natural analogue of Property (iii) of Section 2 holds. The boundedness property (iv) now reads: The unbounded functions $A \in \mathcal{A}$ are bounded on the balls $B^{\le\nu} := \big\{\psi \in \Gamma \;:\; \|\psi\|_2^2 \le \nu\big\}$, with

$$\big\| A(a^{(p)})\big|_{B^{\le\nu}} \big\|_\infty \;\le\; \nu^p\, \|a^{(p)}\|\,. \tag{50}$$

Moreover, all functions in $\mathcal{A}$ are gauge invariant.

4 Quantization

In this section, we interpret the original quantum-mechanical problem as the quantization of the classical Hamiltonian system described in Section 3. Quantization is the linear map $\widehat{(\cdot)}_N : \mathcal{A} \mapsto \widehat{\mathcal{A}}$ defined by the substitution

$$\overline{\psi}(x) \;\mapsto\; \widehat{\psi}_N^*(x)\,, \tag{51a}$$

$$\psi(x) \;\mapsto\; \widehat{\psi}_N(x)\,, \tag{51b}$$

followed by Wick ordering (see (48) and (32)). Note that quantization maps the Poisson bracket $\{\psi^{\#_1}(x), \psi^{\#_2}(y)\}$ to the commutator $iN\big[\widehat{\psi}_N^{\#_1}(x), \widehat{\psi}_N^{\#_2}(y)\big]$, (where a symbol $\#_i$ stands for either complex conjugate, resp. adjoint, or nothing). Furthermore we have, under quantization,

$$\overline{A} \;\mapsto\; \widehat{A}_N^*\,, \tag{52}$$

$$A(a^{(p)}) \;\mapsto\; \widehat{A}_N(a^{(p)})\,, \tag{53}$$

$$\mathscr{H} \;\mapsto\; \widehat{\mathscr{H}_N}\,. \tag{54}$$

[3] Actually global solutions exist for arbitrary $\psi_0 \in L^2(\mathbb{R}^3)$, since Duhamel's formula implies that the map $\psi_0 \mapsto \psi_t$ is L^2-bounded.

Thus, $\mathcal{A}$ is deformed to $\widehat{\mathcal{A}}$, with deformation parameter $1/N$.

Quantization does, of course, not intertwine the quantum-mechanical time evolution with the classical (Hartree) time evolution, *except* when $\phi = 0$. Denoting by Φ_0^t the classical flow for $\phi = 0$, we have the following result.

LEMMA.

$$\text{(a)} \qquad A(a^{(p)}) \circ \Phi_0^t \;=\; A\Big(e^{itH_0^{(p)}}\, a^{(p)}\, e^{-itH_0^{(p)}}\Big)\,, \tag{55}$$

$$\text{(b)} \qquad e^{itN\widehat{\mathscr{H}}_{0,N}}\, \widehat{A}_N(a^{(p)})\, e^{-itN\widehat{\mathscr{H}}_{0,N}} \;=\; \big(A(a^{(p)}) \circ \Phi_0^t\big)\widehat{}_N\,. \tag{56}$$

To conclude this section, we note that the quantization of the continuum theory of gases described by the Hartree equation (Section 3) apparently reproduces the atomistic quantum theory of interacting Bose gases (Section 2), as discussed in Section 1.

5 The Mean-Field Limit, and a Egorov Theorem

Here we state our main result: Quantization intertwines the full quantum-mechanical time evolution with the Hartree evolution *in the mean-field limit.*

THEOREM. *Let $\nu > 0$ be an arbitrary constant and $a^{(p)}$ as above. Then*

$$e^{itN\widehat{\mathscr{H}}_N}\, \widehat{A}_N(a^{(p)})\, e^{-itN\widehat{\mathscr{H}}_N}\Big|_{\mathcal{F}\le \nu N} \;=\; \big(A(a^{(p)}) \circ \Phi^t\big)\widehat{}_N\Big|_{\mathcal{F}\le \nu N} + o(1)\,, \tag{57}$$

as $N \to \infty$.

SKETCH OF PROOF. The proof is based on an expansion of (57) for small times, which is then iterated to obtain the claim for all times. We begin with some comments on notation. The interaction potential can be written as

$$\widehat{\mathscr{V}}_N \;=\; \frac{1}{2}\, \widehat{A}_N(\phi^{(2)})\,, \tag{58}$$

with $\phi^{(2)}(x_1, x_2; y_1, y_2) := \phi(x_1 - y_1)\, \delta(x_2 - y_1)\, \delta(y_2 - x_1)$ and $\|\phi^{(2)}\| = \|\phi\|_\infty$. Denote by

$$a_t^{(p)} \;:=\; e^{itH_0^{(p)}}\, a^{(p)}\, e^{-itH_0^{(p)}} \tag{59}$$

the operator $a^{(p)}$ evolved to time t, using the one-particle dynamics. We expand the left-hand side of (57) by using the above lemma:

$$\begin{aligned} e^{itN\widehat{\mathscr{H}}_N}\, \widehat{A}_N(a^{(p)})\, e^{-itN\widehat{\mathscr{H}}_N} \;&=\; \widehat{A}_N(a_t^{(p)}) \\ &+ \int_0^t ds\, e^{isN\widehat{\mathscr{H}}_N}\, e^{-isN\widehat{\mathscr{H}}_{0,N}}\, \frac{iN}{2}\big[\widehat{A}_N(\phi_s^{(2)}), \widehat{A}_N(a_t^{(p)})\big]\, e^{isN\widehat{\mathscr{H}}_{0,N}}\, e^{-isN\widehat{\mathscr{H}}_N}\,. \end{aligned} \tag{60}$$

Iteration of this identity yields a Schwinger-Dyson series that converges for all times t, but with convergence estimates in N that become useless as $N \to \infty$. A look at the commutator

$$\frac{iN}{2}\big[\widehat{A}_N(\phi_s^{(2)}), \widehat{A}_N(a_t^{(p)})\big] \;=\; \sum_{l=1}^{2} \binom{p}{l}\binom{2}{l} \frac{il}{2N^{l-1}}\, \widehat{A}_N\Big(\big[(\phi_s^{(2)}) \underset{l}{\rightharpoonup} (a_t^{(p)})\big]\Big) \tag{61}$$

suggests splitting the iterated series into two parts. As we iterate (60) we generate "tree terms" ($l = 1$) and "loop terms" ($l = 2$). As soon as a loop term is generated, we stop expanding and put it into an error term of order $1/N$. Thus we get

$$e^{itN\widehat{\mathscr{H}_N}}\, \widehat{A}_N(a^{(p)})\, e^{-itN\widehat{\mathscr{H}_N}} \;=\; \widehat{T}(a^{(p)},t) + \widehat{R}(a^{(p)},t)\,, \tag{62}$$

where

$$\begin{aligned}\widehat{T}(a^{(p)},t) \;&:=\; \sum_{k=0}^{\infty} i^k\,(p+k-1)(p+k-2)\cdots p \int_0^t dt_1 \int_0^{t_1} dt_2 \ldots \int_0^{t_{k-1}} dt_k \\ &\qquad\qquad \cdot\,\widehat{A}_N\Big(\Big[\phi^{(2)}_{t_k} \underset{1}{\rightharpoonup} \big[\phi^{(2)}_{t_{k-1}} \underset{1}{\rightharpoonup} \ldots [\phi^{(2)}_{t_1} \underset{1}{\rightharpoonup} a^{(p)}_t]\big]\Big]\Big)\end{aligned} \tag{63}$$

and

$$\begin{aligned}\widehat{R}(a^{(p)},t) \;&:=\; \sum_{k=0}^{\infty} \frac{i^{k+1}}{2N}\,(p+k)(p+k-1)\cdots p\,(p+k-1) \int_0^t dt_1 \int_0^{t_1} dt_2 \ldots \int_0^{t_k} dt_{k+1} \\ &\quad \cdot\, e^{it_{k+1}N\widehat{\mathscr{H}_N}}\, e^{-it_{k+1}N\widehat{\mathscr{H}_{0,N}}}\, \widehat{A}_N\Big(\Big[\phi^{(2)}_{t_{k+1}} \underset{2}{\rightharpoonup} \big[\phi^{(2)}_{t_k} \underset{1}{\rightharpoonup} \ldots [\phi^{(2)}_{t_1} \underset{1}{\rightharpoonup} a^{(p)}_t]\big]\Big]\Big) \\ &\qquad\qquad \cdot\, e^{it_{k+1}N\widehat{\mathscr{H}_{0,N}}}\, e^{-it_{k+1}N\widehat{\mathscr{H}_N}}\,.\end{aligned} \tag{64}$$

Using the bound (38) it is not hard to see that, on the subspace $\mathcal{F}^{\leq \nu N}$, both series converge absolutely if

$$|t| \;\leq\; \frac{1}{4\nu\|\phi\|_\infty}\,. \tag{65}$$

Note that one could only stop expanding after M loops have been generated (instead of $M = 1$ here), thus getting a systematic $1/N$-expansion of the form

$$\begin{aligned}&e^{itN\widehat{\mathscr{H}_N}}\, \widehat{A}_N(a^{(p)})\, e^{-itN\widehat{\mathscr{H}_N}} \\ &\qquad =\; \widehat{T}(a^{(p)},t) + \widehat{L}_1(a^{(p)},t) + \cdots + \widehat{L}_M(a^{(p)},t) + \widehat{R}_M(a^{(p)},t)\,,\end{aligned} \tag{66}$$

where, on $\mathcal{F}^{\leq \nu N}$, the "m-loop term" $\widehat{L}_m$ is of order N^{-m}. All terms converge absolutely provided that $|t|$ is smaller than the convergence radius given in (65).

In order to make the link with the Hartree time evolution we expand the right-hand side of (57) in a Schwinger-Dyson series (a subscript time index on an observable again denotes free time evolution):

$$A(a^{(p)}) \circ \Phi^t \;=\; \sum_{k=0}^{\infty} \int_0^1 dt_1 \ldots \int_0^{t_{k-1}} dt_k \,\Big\{\mathscr{V}_{t_k}, \{\mathscr{V}_{t_{k-1}}, \ldots \{\mathscr{V}_{t_1}, A(a^{(p)}_t)\}\}\Big\}\,. \tag{67}$$

Using

$$\big\{A(a^{(p)}), A(b^{(q)})\big\} \;=\; ipq A\big(\big[a^{(p)} \underset{1}{\rightharpoonup} b^{(q)}\big]\big) \tag{68}$$

(no loop terms are generated for the classical dynamics), as well as $\mathscr{V} = A(\phi^{(2)})/2$, we find that

$$\begin{aligned}A(a^{(p)}) \circ \Phi^t \;&=\; \sum_{k=0}^{\infty} i^k\,(p+k-1)(p+k-2)\cdots p \int_0^t dt_1 \int_0^{t_1} dt_2 \ldots \int_0^{t_{k-1}} dt_k \\ &\qquad\qquad \cdot\, A\Big(\Big[\phi^{(2)}_{t_k} \underset{1}{\rightharpoonup} \big[\phi^{(2)}_{t_{k-1}} \underset{1}{\rightharpoonup} \ldots [\phi^{(2)}_{t_1} \underset{1}{\rightharpoonup} a^{(p)}_t]\big]\Big]\Big)\,.\end{aligned} \tag{69}$$

As above, using (50), it is easy to show that the series converges absolutely on $B^{\leq \nu}$ if $|t| < (4\nu \|\phi\|_\infty)^{-1}$. Quantization and comparison with (63) proves the claim for $|t| < (4\nu \|\phi\|_\infty)^{-1}$.

To iterate these expansions, it is crucial that the convergence radius (65) is independent of p, so that each term of (63) may be iterated by a time step $\tau < (4\nu \|\phi\|_\infty)^{-1}$. A priori, the error term $\widehat{R}$ is not uniformly bounded in p, so that a cutoff in k is necessary. Given $\varepsilon > 0$, we choose K large enough that the tail $k > K$ of (63) is bounded by ε, and expand each term with $k \leq K$. All loop terms are put into an error term. We continue iteratively in this fashion for a finite number s of steps and reach all times $t \leq s\tau$. As the number of loop terms increases at each iteration, we choose $\varepsilon = \varepsilon(N)$, with $\varepsilon(N) \to 0$, as $N \to \infty$, sufficiently slowly to guarantee the vanishing of the error term in the limit $N \to \infty$. The bound so obtained is weaker than the $1/N$-estimate obtained for short times. We repeat a similar analysis for the classical expansion. As before, the claim follows by comparing the quantized classical expansion with the quantum-mechanical one. □

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