Classical Statistics as a Limiting Case of Quantum Statistics

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Dedicated to Professor Pascual Jordan *on the occasion of his 65th birthday*

The scope of validity of the quantum mechanical *correspondence principle* is discussed: for what classes of Hamilton functions does canonical quantization give rise to a quantum theory whose equilibrium predictions tend towards the classical ones in the limit of large energies? As the rule for *canonical quantization* we adopt the Weyl–Wigner map (of real phase space functions onto selfadjoint Hilbert space operators) which appears to be the simplest that guarantees *commutability* of quantization with continuous *coordinate change* in position space. Counterexamples show that there is *no general validity* of a correspondence principle. On the other hand, such a principle is known to hold for all physically reasonable cases.

1. Introduction

Quantum mechanics has been founded as a refinement of classical mechanics mainly for low energies (small particle numbers). In the limit of *high energies,* quantum formulae have to tend towards their classical counterparts. Especially, Boltzmann *statistics* has to tend towards Gibbs *statistics* for particle energies large compared with some characteristic energy $k\,T_0$. Which can be stated, e. g. as an asymptotic equality of the partition sums $Z(T)$ of the respective statistics. They are defined as

$$Z_{\mathrm{G}}(\beta) := \int \mathrm{d}m\; e^{\beta H(p,q)}, \quad \beta := -1/k\,T, \tag{1}$$

$$Z_{\mathrm{B}}(\beta) := \sum_j w_j\, e^{\beta H_j}, \tag{2}$$

where the indices G and B stand for "Gibbs" and "Boltzmann", $H(p,q)$ is Hamilton's *energy* function on $2\,f$-dim *phase space* with volume element

$$\mathrm{d}m := h^{-f} \prod_j \mathrm{d}p_j \prod_k \mathrm{d}q_k\,, \quad (h = \text{Planck's constant}), \tag{3}$$

and where H_j stands for the eigenvalues of the corresponding Hamilton operator, and w_j for the dimension of the eigen space belonging to H_j (called its *statistical weight*).

The partition integral Z_{G} can also be written as a one-dim energy integral

$$Z_{\mathrm{G}}(\beta) = \int \mathrm{d}H\, m'(H)\, e^{\beta H}\,, \tag{4}$$

which is approximated by the sum (2) if $w_j\, e^{\beta H_j}$ approximates the integrand $m'(H)\, e^{\beta H}$ up to a constant factor. The latter is similar in shape to $H^f\, e^{-|\beta| H}$ whose essential support is a "thin" neighbourhood of the energy surface $H = f/|\beta| = f\,k\,T$. Consequently, Z_{B} approaches Z_{G} for large energies if $w_j =: w(H_j)$ approaches $\mathrm{d}m(H_j)$ for $H_j \gg f\,k\,T_0$. In words: quantum statistics approaches classical statistics for large energies if the eigenvalue density, or *statistical weight* of the *energy shell* approaches its *volume* (measured in units of h^f).

Such an asymptotic equality is inherent in Bohr's heuristic *quantization rule*

$$\oint p_k\, \mathrm{d}q_k = n\,h \tag{5}$$

which implies for one-dim systems that neighbouring "quantum orbits" divide phase space into cells of constant volume h. It is the purpose of the present paper to investigate the *scope* of its *validity* for arbitrary Hamilton functions quantized according to the Weyl–Wigner correspondence.

The correspondence of Weyl and Wigner gives a *quantization rule* Φ which is *invariant* under continuous coordinate changes in position space. That is

$$\Phi : H(p,q) \to \mathbf{H} \tag{6}$$

is a mapping of real phase space functions $H(p,q)$ onto selfadjoint Hilbert space operators $\mathbf{H}$ which defines a Hamilton operator $\mathbf{H}$ for every Hamilton function H such that continuously related position space descriptions give rise to unitarily related quantum theories; proofs are given in [1]. This rule is of course not unique (because of the freedom to perform unitary transformations), but it is the simplest rule known to me. Its properties will be described in section 2, and used for a comparison of the statistical weight with the energy shell volume in section 3.

[1] W. Kundt, Springer Tracts in Modern Physics **40**, 107 [1966].

2. Canonical Quantization

In this section we summarize the relevant properties of the *invariant quantization rule* Φ suggested by WEYL, and used by WIGNER (and many others) for a phase space description of a quantized system (proofs and references are given in [1]).

Φ is conveniently introduced as a mapping of *square integrable* (complex) phase space functions $H(p, q)$ onto *trace operators* $\mathbf{H}$ in HILBERT space $[\mathrm{tr}(\mathbf{H}^* \mathbf{H}) < \infty]$, which is based upon FOURIER transformations. As such it is a *linear isomorphism* which maps the *phase space scalar product*

$$\langle A, B \rangle := \int \mathrm{d}m\, A^*(p, q)\, B(p, q) \tag{7}$$

onto the *operator scalar product*

$$\langle \mathbf{A}, \mathbf{B} \rangle := \mathrm{tr}(\mathbf{A}^* \mathbf{B}), \quad (\mathbf{A}^* := \mathrm{adjoint}(\mathbf{A})). \tag{8}$$

In other words, Φ is a HILBERT *space isomorphism.* Moreover, its inverse Φ^{-1} maps the *commutator* of operators

$$[\mathbf{A}, \mathbf{B}] := (i/\hbar)(\mathbf{A}\mathbf{B} - \mathbf{B}\mathbf{A}) \tag{9}$$

onto the MOYAL *bracket* of phase space functions:

$$[A, B] := (2/\hbar)\sin(\tfrac{1}{2}\hbar\Gamma)\, A\, B. \tag{10}$$

Here, Γ is the POISSON operator which maps two functions A, B onto their POISSON *bracket*

$$[A, B]_{\mathrm{P}} := \Gamma A B := \sum_j (\overset{A}{\partial}_{pj}\overset{B}{\partial}_{qj} - \overset{A}{\partial}_{qj}\overset{B}{\partial}_{pj})\, A\, B, \tag{11}$$

where an upper kernel index A says that this differentiation operator acts on the function A only. Like the commutator, the MOYAL bracket (10) is a LIE *product.* It is *non-local* because it is formed from the second order differential operator Γ by insertion into the (infinite) power series expansion of the sine-function. However, the MOYAL bracket differs from the POISSON bracket by terms of second degree in $\hbar$ only, and is identical with it if A or B are polynomials of maximal degree two in p_j and q_k. Consequently, Φ is also a LIE *algebra isomorphism* (whenever the LIE product is defined) if one uses the MOYAL bracket as a LIE product on the phase space functions.

In what follows, we do not need the definition of Φ (which is lengthy). Instead we observe that Φ can be extended to arbitrary *analytic functions,* and that this unique extension is given by ($[\mathbf{P}_j, \mathbf{Q}_k] = \delta_{jk}$ for the commutator defined in (9))

$$\Phi A = \exp\{-\tfrac{1}{2} i\hbar \sum_j \partial_{\mathbf{P}_j}\partial_{\mathbf{Q}_j}\}\, A_{\mathrm{L}}(\mathbf{P}, \mathbf{Q}); \tag{12}$$

here the *left ordered* operator $A_{\mathrm{L}}(\mathbf{P}, \mathbf{Q})$ is obtained from the power series $A(p, q)$ by replacing all p_j, q_k by their corresponding operators $\mathbf{P}_j$, $\mathbf{Q}_k$ such that all the $\mathbf{Q}_j$'s stand to the left of the $\mathbf{P}_k$'s. As an immediate consequence one sees that functions of the p_j's or q_k's alone are mapped under Φ onto the same functions of the corresponding operators:

$$\Phi A(p) = A(\mathbf{P}), \quad \Phi A(q) = A(\mathbf{Q}). \tag{13}$$

We remark that the effect of the map (12) is to replace polynomials by their corresponding *totally symmetrized* operator polynomials.

For later use we mention the following example calculated from (12)

$$\begin{aligned}\Phi(p\,q^2)^2 &= \mathbf{Q}^4\mathbf{P}^2 - 4i\hbar\mathbf{Q}^3\mathbf{P} - 3\hbar^2\mathbf{Q}^2 \\ &= \tfrac{1}{4}(\mathbf{Q}^2\mathbf{P} + \mathbf{P}\mathbf{Q}^2)^2 - 2\hbar^2\mathbf{Q}^2.\end{aligned} \tag{14}$$

3. Discussion of Asymptotic Equality

In order to compare the statistical weight w_j introduced in (2) with the energy shell volume $\mathrm{d}m(H)$, we have to translate the quantum mechanical eigen value problem into phase space language. The *energy eigen value* problem reads

$$\mathbf{H}\mathbf{E}_j = H_j \mathbf{E}_j, \tag{15}$$

where H_j are the (real) eigen values of the (selfadjoint) HAMILTON operator $\mathbf{H}$, and $\mathbf{E}_j$ the projection operators on the corresponding eigen spaces:

$$\mathbf{E}_j^2 = \mathbf{E}_j, \quad \mathbf{E}_j^* = \mathbf{E}_j, \quad \mathrm{tr}(\mathbf{E}_j) = w_j; \tag{16}$$

by definition, w_j are the dimensions of the eigen spaces, hence equal to the traces of the projection operators. Equation (15) can be decomposed into its *selfadjoint* and *antiselfadjoint* part:

$$[\mathbf{H}, \mathbf{E}_j] = 0, \quad \mathbf{H}\mathbf{E}_j + \mathbf{E}_j\mathbf{H} = 2H_j\mathbf{E}_j. \tag{17}$$

Under the WEYL–WIGNER correspondence described in section 2, Eqs. (17) map into the following *phase space equations* [compare (10), (11)]

$$[H, E_j] = 0, \tag{18}$$

and

$$\cos(\tfrac{1}{2}\hbar\Gamma)\, H(p, q)\, E_j(p, q) = H_j E_j(p, q). \tag{19}$$

Here $H(p, q)$ is (as always) the HAMILTON function, and $E_j(p, q)$ is the phase space image of the projection operator $\mathbf{E}_j$. If in Eq. (18) the MOYAL bracket is replaced by the POISSON bracket, this equation says that E_j must be a *constant* of the *motion.* In the simplest case of the one-dim harmonic oscillator, this replacement is admissible, and E_j must be a function of H. In this case, Eq. (19) becomes an ordinary differential equation for $E_j(H)$.

Let us assume that the operator $\mathbf{H}$ has a *pure point spectrum.* In this case, the spectral theorem says that $\sum_{j=-\infty}^{J} \mathbf{E}_j$ converges weakly (in the trace norm) towards the unit operator for $J \to \infty$, which implies that $\sum_{j=-\infty}^{J} E_j$ converges weakly (in the L^2 norm) towards the *unit function* on phase space. We have [compare (8)]

$$w_j = \begin{cases} \langle \mathbf{E}_j, \mathbf{1} \rangle = \langle E_j, 1 \rangle, \text{ and} \\ \langle \mathbf{E}_j, \mathbf{E}_j \rangle = \langle E_j, E_j \rangle, \end{cases} \tag{20}$$

which shows that E_j is a *square integrable* function for $w_j < \infty$ whose *integral* is equal to w_j.

On the other hand, the measure $\mathrm{d}m = \mathrm{d}H\, m'(H)$ of the *energy shell* of thickness $\mathrm{d}H$ can be written as

$$\mathrm{d}m = \langle \chi_{\mathrm{d}H}, 1 \rangle \tag{21}$$

where $\chi_{\mathrm{d}H}(p, q)$ is the characteristic function of the shell. Consequently

$$\mathrm{d}_j m - w_j = \langle \chi_j - E_j, 1 \rangle, \tag{22}$$

so that asymptotic equality of the statistical weight w_j and the shell volume $\mathrm{d}_j m$ is guaranteed if there exists a shell decomposition of phase space such that E_j converges (in the L^1 norm) towards the characteristic function χ_j of the j-th shell (around H_j) for $H_j \to \infty$.

Such a *convergence* actually occurs for physically reasonable Hamilton functions, for the following reason: We have already seen that $\{E_j\}$ is a decomposition of the unit function; that is $\sum_j E_j = 1)$. If moreover the function E_j is essentially *supported* by a shell of decreasing thickness around $H(p, q) = H_j$ (i. e. if it is negligibly small outside of such a shell), this decomposition is essentially a shell decomposition with centers H_j.

The support property just mentioned is a consequence of Eq. (19). In order to get an intuitive understanding, let us consider the *harmonic oscillator* for which $\Gamma^3 H A = 0$ so that (19) simplifies to

$$\tfrac{1}{8}\hbar^2 H^{-1} \Gamma^2 H E_j = (1 - H_j/H)\, E_j. \tag{23}$$

H is by assumption a quadratic form, which implies that the left hand side is (in suitable coordinates) equal to the Laplacian applied to E_j. The parenthesis on the right hand side assumes large negative values for $H < H_j$, and tends towards 1 for $H > H_j$. As a consequence, E_j oscillates strongly for $H < H_j$, becomes large for $H \approx H_j$, and decreases exponentially for $H > H_j$. In the limit $H_j \to \infty$, the essential support of E_j shrinks to the sphere $H = H_j$.

We do not attempt to derive quantitative statements about the eigenvalue distribution w_j; for Hamilton operators of the general form

$$\mathbf{H} = \vec{\boldsymbol{P}}\, F(\vec{\boldsymbol{Q}})\, \vec{\boldsymbol{P}} + G(\vec{\boldsymbol{Q}})$$

this has been done in [2]. Instead we want to show that without any proviso there are obvious *counter examples* to an asymptotic convergence. For instance it can happen that the Hamilton operator $\mathbf{H}$ has a continuous (part of the) spectrum so that the place of the spectral operators $\mathbf{E}_j$ is taken by projection operators on infinite dimensional subspaces. The corresponding statistical heights w_j are infinite. One might conjecture that in this case the volume of the energy shell was likewise infinite, in agreement with the fact that continuous spectra occur in dissociated (ionized) systems whose orbits (in phase space) extend to infinity. However there are Hamilton functions with *bounded energy surfaces* whose associated operators have a *continuous spectrum!* Similarly one might conjecture that a *positive* function gave rise to an operator *bounded* from below, or that a *positive* operator gave rise to a function *bounded* from below. The last conjecture is refuted by the hydrogen atom, and the former one will be likewise disproven.

To this end consider the function

$$H = (p\, q^2)^2 + \alpha (p^2 + q^2), \quad \alpha \geqq 0. \tag{24}$$

H is evidently positive, and the surfaces $H = \text{const}$ are bounded for every $\alpha > 0$. I am going to prove that its corresponding operator $\mathbf{H}$ is *unbounded* to either side for sufficiently small α, and has a *continuous* spectrum for $\alpha < 7\hbar^2/4$. First of all, from Eq. (14) we have

$$\begin{aligned} \mathbf{H} := \Phi H &= (\mathbf{Q}^4 + \alpha)\mathbf{P}^2 - 4 i \hbar\, \mathbf{Q}^3 \mathbf{P} + (\alpha - 3\hbar^2)\, \mathbf{Q}^2 \\ &= \tfrac{1}{4}(\mathbf{Q}^2 \mathbf{P} + \mathbf{P} \mathbf{Q}^2)^2 + \alpha \mathbf{P}^2 - (2\hbar^2 - \alpha)\, \mathbf{Q}^2. \end{aligned} \tag{25}$$

The second line shows that $\mathbf{H}$ is the difference of two positive unbounded selfadjoint operators, which hints at non-boundedness. Let us evaluate the diagonal matrix element $(f, \mathbf{H} f)$ in the position representation where $f = f(q)$, $\mathbf{Q}$ acts as multiplication by q,

[2] R. Courant and D. Hilbert, Methoden der Mathematischen Physik I, Springer, Berlin 1931; see Chapter VI, § 4.

and $\mathbf{P}$ as differentiation $-i\hbar\,\partial$, $(\partial := \partial_q)$; and let us content ourselves with the special case $\alpha = 0$

$$\hbar^{-2}(f, \mathbf{H} f) = \| \tfrac{1}{2}(q^2\,\partial + \partial q^2)\, f \|^2 - 2 \, \| q f \|^2 = \int \mathrm{d}q\; q^2 \{ | q f' + f |^2 - 2 \, | f |^2 \} . \quad (26)$$

It is not difficult to see that there are functions $f(q)$ of norm 1 for which the integral in (26) assumes arbitrarily large positive or negative values: In the first case one has to choose $|f'|$ large for large $|q|$ whereas in the second case one may choose f like a table mountain profile.

In order to see that $\mathbf{H}$ in (25) has *continuous spectrum* for $\alpha < 7\,\hbar^2/4$, we consider its eigen value equation in the position representation

$$\begin{aligned} 0 &= (\mathbf{H} - H_j)\, f_j \\ &= -\hbar^2 (q^4 + \alpha) \{ \partial^2 + 4\, q^{-1} (1 + \alpha\, q^{-4})^{-1}\, \partial + 3\, q^{-2} (1 + \alpha\, q^{-4})^{-1} (1 - \alpha/3\,\hbar^2 + H_j\, q^{-2}/3\,\hbar^2) \}\, f_j \end{aligned} \quad (27)$$

which becomes asymptotically for large $|q|$

$$0 \cong \{ \partial^2 + 4\, q^{-1}\, \partial + 3\, q^{-2} (1 - \alpha/3\,\hbar^2) \}\, f . \quad (28)$$

Here we have written f for f_j because the eigen value H_j does not enter into the asymptotic form. Eq. (28) can be solved in closed form by means of a power ansatz:

$$f \cong c\, q^\gamma \quad \text{with} \quad \gamma = -\tfrac{3}{2} \pm \sqrt{\alpha/\hbar^2 - \tfrac{3}{4}} . \quad (29)$$

This is the asymptotic form of all eigen functions for $|q| \to \infty$, where the two signs of the square root correspond to the two linearly independent solutions. If both of them are square integrable, so are all solutions of Eq. (27), and the spectrum contains all the reals. This happens for $\gamma < -1/2$, or $\alpha/\hbar^2 < 7/4$ as has been claimed above.

Erweiterte Gravitationstheorie, Machsches Prinzip und rotierende Massen

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The rotation of the local inertial frames induced by a rotating shell of mass is calculated in the framework of P. JORDAN's "extended theory of gravitation". As a special case, the corresponding results are obtained for BRANS and DICKE's "scalar-tensor" theory. In the weak field approximation the result is the same as the LENSE–THIRRING effect of General Relativity, except for a factor depending on the coupling constant of the scalar field. The strong field limit in which the inertial frame is completely dragged along by the rotating shell is investigated. In particular it is shown that this limit of perfect dragging occurs in certain cosmological models whenever the density of the rest of the matter in the universe tends to zero. This result is interpreted as a manifestation of MACH's principle in the extended theory of gravitation.

Das wachsende Interesse an der JORDANschen erweiterten Gravitationstheorie [1a] beruht einerseits auf einer Anzahl experimenteller Tatsachen, die auf eine zeitlich und räumlich veränderliche Gravitations-„konstante" hinweisen [1b] und andererseits auf den anziehenden mathematischen Eigenschaften dieser natürlichen Verallgemeinerung der EINSTEINschen Gravitationstheorie. So haben z. B. BRANS und DICKE besonders hervorgehoben, daß bei geeigneter Parameterwahl die JORDANsche Theorie eine gewisse Form des MACHschen Prinzips erfüllt [2]. Leider ist das MACHsche Prinzip heute immer noch eine heuri-

[1a] Unter der „erweiterten Gravitationstheorie" verstehen wir die zuerst von JORDAN [1b] aufgestellten Gleichungen, die die Gravitationserscheinungen als Auswirkung einer pseudo-RIEMANNschen Metrik und eines skalaren Feldes erklären. Bis auf geringe Unterschiede der Bezeichnung ist diese Theorie identisch mit DICKES [1b] „Skalar-Tensor"-Theorie. Da der Fragenkreis der vorliegenden Arbeit nur mit der erweiterten Gravitationstheorie zu tun hat, wollen wir hier auf den übrigen Teil der JORDANschen Theorie (z. B. die Theorie der Sternentstehung und die Theorie der Erdexpansion) nicht weiter eingehen.

[1b] Siehe z. B. P. JORDAN, Schwerkraft und Weltall, Friedr. Vieweg & Sohn, Braunschweig 1955, § 34. — P. JORDAN, Problems of Gravitation—Empirical Aspects of DIRAC's Hypothesis, Office of Aerospace Res. Rep. 1961. — R. H. DICKE, Physics Today **20**, 55 [1967]. — R. H. DICKE u. H. M. GOLDENBERG, Phys. Rev. Letters **18**, 318 [1967].

[2] C. BRANS u. R. H. DICKE, Phys. Rev. **124**, 925 [1961].