ON THE CLASSICAL LIMIT OF QUANTUM MECHANICS

By W. Siegel

Institute of Physics, Jagellonian University, Cracow*

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The classical limit of nonrelativistic quantum mechanics in the Wigner phase-space formalism is discussed. It appears that the limit of an eigenstate is represented by a singular probability density concentrated and constant on subsets of phase space corresponding to the given value of the observable. The limit of eigenstates of energy is investigated as an example.

1. *Introduction*

The purpose of this paper is to discuss the "classical limit" of nonrelativistic quantum mechanics using the Wigner phase-space representation. This formalism, developed by Wigner [1], Groenewold [2] and Moyal [3, 4] seems to be best-suited for comparing quantum and classical theories. In spite of this, to the knowledge of the author, no more extensive discussion of this kind can be found in the literature, and more complicated methods are preferred (e.g. Maslov [5]).

We shall restrict our attention to the theory of one spinless particle moving in one dimension. Generalization to more translational degrees of freedom should be simple. Spin may be included in a way described in [6–8].

We start with reminding some basic facts from the Wigner phase-space formalism, to fix the conventions and notation. The operators acting in the Hilbert space of states will be distinguished by using bold-faced type throughout the paper. Other letters denote c-numbers.

The operator

$$\Delta(q, p) = \frac{1}{h}\int du dw \exp\left[\frac{i}{\hbar}(u(\mathbf{q}-q)+w(\mathbf{p}-p))\right]$$

* Address: Instytut Fizyki UJ, Reymonta 4, 30-059 Kraków, Poland.

enables us to define the Wigner representation of any operator $\boldsymbol{A}$ (including the density operator):

$$A(q, p) = \mathrm{Tr}\,(\boldsymbol{A} \cdot \boldsymbol{\Delta}(q, p))$$
$$= \hbar \int du e^{ipu} \left\langle q - \frac{\hbar u}{2} \right| \boldsymbol{A} \left| q + \frac{\hbar u}{2} \right\rangle. \tag{1}$$

Conversely,

$$\boldsymbol{A} = \frac{1}{h} \int dq dp \boldsymbol{\Delta}(q, p) A(q, p)$$

and for the quantum average we have

$$\mathrm{Tr}\,(\boldsymbol{\varrho} \cdot \boldsymbol{A}) = \frac{1}{h} \int dq dp A(q, p) f(q, p), \tag{2}$$

where $\boldsymbol{\varrho}$ is the density operator and $f(q, p)$ its Wigner representation. The normalization condition is

$$\frac{1}{h} \int dq dp f(q, p) = 1. \tag{3}$$

The Groenewold rule provides us with the phase representation $C(q, p)$ of the product $\boldsymbol{C} = \boldsymbol{A} \cdot \boldsymbol{B}$ of two operators $\boldsymbol{A}$ and $\boldsymbol{B}$:

$$C(q, p) = A(q, p) \exp\left(\frac{i\hbar}{2} \Lambda\right) B(q, p), \tag{4}$$

where

$$\Lambda = \frac{\overleftarrow{\partial}}{\partial q} \cdot \frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p} \cdot \frac{\overrightarrow{\partial}}{\partial q},$$

the arrows indicating the direction in which the derivatives operate. Thus the von Neumann evolution equation reads

$$\frac{\partial}{\partial t} f(q, p, t) = H(q, p) \frac{2}{\hbar} \sin\left(\frac{\hbar}{2} \Lambda\right) f(q, p, t). \tag{5}$$

$H(q, p)$ is the Wigner representation of the Hamiltonian.

2. *Observables*

Consider a classical dynamical quantity of the form:

$$A_{\mathrm{cl}}(q, p) = \sum_{n,m \geqslant 0} a_{nm} q^n p^m.$$

According to the standard procedure of quantization the corresponding quantum observable is

$$\boldsymbol{A} = \sum_{n,m \geqslant 0} a_{nm} (\boldsymbol{q}^n \cdot \boldsymbol{p}^m)_{\mathrm{ord}},$$

where the bracket indicates some specific rule of ordering of the noncommuting operators $\boldsymbol{q}$ and $\boldsymbol{p}$. With the aid of a finite number of commutations we transform $(\boldsymbol{q}^n \cdot \boldsymbol{p}^m)_{\text{ord}}$ into the Weyl-ordered product $(\boldsymbol{q}^n \cdot \boldsymbol{p}^m)_{\text{W}}$ [9]:

$$(\boldsymbol{q}^n \cdot \boldsymbol{p}^m)_{\text{ord}} = (\boldsymbol{q}^n \cdot \boldsymbol{p}^m)_{\text{W}} + \hbar \text{ (remaining terms)},$$

the (remaining terms) being a polynomial in $\hbar$.

The Wigner representation of $(\boldsymbol{q}^n \cdot \boldsymbol{p}^m)_{\text{W}}$ is $q^n \cdot p^m$, so

$$A(q, p) = A_{\text{cl}}(q, p) + \hbar \text{ (other terms)}$$

and

$$\lim_{\hbar \to 0} A(q, p|\hbar) = A_{\text{cl}}(q, p).$$

Similar results were obtained by A. S. Schwartz [10]. From (4) we see that in the limit $\hbar \to 0$ the Groenewold product becomes the ordinary product $A \cdot B$. Thus the algebra of quantum observables having classical counterparts tends to the "classical algebra of observables".

3. *Classical limit of a quantum state*

We almost always specify the state of a system giving the expansion of its density operator in terms of eigenvectors of an observable (some commuting observables). Therefore we shall restrict our considerations to eigenstates of observables which possess classical limit.

Let $|\Psi\rangle$ be an eigenvector of such an observable A to an eigenvalue a. Thus

$$f_\Psi = \langle \Psi | \Delta(q, p) | \Psi \rangle = f(q, p | \hbar, a).$$

Before performing the limit $\hbar \to 0$ we must determine the dependence of a on $\hbar$.

For a taking on discrete values we may define two "classical limits" in a natural way:

(a) we fix the number n of the eigenvalue $a_n(\hbar)$:

$$f_{\text{lim},n}(q, p) = \lim_{\hbar \to 0} \frac{1}{h} f_n(q, p | \hbar, a_n(\hbar)),$$

the factor $\frac{1}{h}$ is due to our normalization convention (3),

(b) $\hbar \to 0$ and $n \to \infty$ so that $a_n(\hbar)$ tends to a given number a:

$$f_{\text{lim},a}(q, p) = \lim_{\hbar \to 0, n \to \infty} \frac{1}{h} f_n(q, p | \hbar, a_n(\hbar)).$$

The limit phase density in (a) may be interpreted as a macroscopic (classical scale measuring devices) description of a microscopic (low quantum numbers) quantum state. Case (b) explains the "quantum nature" of a classical state — the way in which quantum mechanics transforms into classical (statistical) mechanics in the region of applicability of the latter.

If the spectrum of a is continuous there is only one natural definition of the limit

$$f_{\text{lim},a}(q, p) = \lim_{\hbar \to 0, a=\text{const}} \frac{1}{h} f_a(q, p|\hbar).$$

Note that we normalize the eigenstates in the following way

$$\langle a|a'\rangle = h \cdot \delta(a-a') \tag{6}$$

4. Examples

For eigenstates of the position operator

$$f_x(q, p|\hbar) = h\delta(q-x)$$

and as we should expect we get in the limit a classical ensemble of particles with fixed position and arbitrary momentum. For the n-th energy eigenstate of harmonic oscillator [4]

$$f_n(q, p|\hbar) = 2(-1)^n \exp\left(-\frac{2H}{\hbar\omega}\right) L_n\left(\frac{4H}{\hbar\omega}\right),$$

$L_n(x)$ is the Laguerre polynomial and $H(q, p) = H_{\text{cl}}(q, p)$ is the representation of the Hamiltonian.
Limit in the case (a): taking the Fourier transform of f_n, performing the limit and transforming the result back into the phase space we obtain

$$f_{\text{lim},n}(q, p) = \delta(q)\delta(p)$$

(limit in the sense of Schwartz distributions) — the particle resting at the minimum of the potential.

Limit in the case (b): let $E = n\hbar\omega = \text{const}$. The Laplace transform of $\frac{1}{h} f_n$ with respect to $\frac{4H}{E}$ is

$$\frac{2\omega}{E}(-1)^n \left(\frac{s}{n} - \tfrac{1}{2}\right)^n \left(\frac{s}{n} + \tfrac{1}{2}\right)^{-n-1}.$$

The limit $n \to \infty$ and inverse transform give

$$f_{\text{lim},E}(q, p) = \omega\delta(H(q, p)-E)$$

— the microcanonical ensemble for the classical oscillator. Now consider energy eigenstates in a potential well with infinitely high walls at $q = 0$ and $q = d$.

In case (a) we easily calculate using (1) that

$$f_{\text{lim},n}(q, p) = \frac{2}{d}\,\theta(q)\theta(d-q)\sin^2\left(\frac{n\pi q}{d}\right)\delta(p),$$

$\theta(x)$ is the unit step function.

The particle rests but the distribution in space exhibits traces of the "quantum origin". In case (b) let $E_n(\hbar) \to \frac{1}{2m} p_0^2$. From (1) and Riemann–Lebesgue lemma

$$f_{\mathrm{lim},p_0}(q,p) = \frac{1}{2d}\theta(q)\theta(d-q)\,(\delta(p-p_0)+\delta(p+p_0))$$

— again a microcanonical ensemble.

Finally for the coherent states $|z\rangle$, $z = \frac{cq_0+ip_0}{\sqrt{2\hbar c}}$, $f_z(q,p)$ is Gaussian in q, p and

$$f_{\mathrm{lim}}(q,p) = \delta(q-q_0)\delta(p-p_0). \tag{7}$$

5. *General properties of the limit density*

In this section we *assume* that the limit of $\frac{1}{h} f(q,p)$ exists and all the limiting procedures make sense. We list some properties of the limit density $f_{\mathrm{lim}}(q,p)$:

1) according to (3) f_{lim} is normalized to 1 with respect to the measure $dqdp$,

2) f_{lim} is real and positive definite

$$0 \leqslant \frac{1}{h}\langle z|\varrho|z\rangle = \frac{1}{h^2}\int dqdpf(q,p)f_z(q,p) \to f_{\mathrm{lim}}(q_0,p_0).$$

We used here (2) and (7),

3) if f represents a pure state we have

$$\frac{1}{h^2} f \exp\left(\frac{i\hbar}{2}\Lambda\right) f = \frac{1}{h^2} f.$$

In the limit $h \to 0$ we obtain $(f_{\mathrm{lim}}(q,p))^2 = \infty$ if only $f_{\mathrm{lim}}(q,p) \neq 0$. Thus the limit of $\frac{1}{h} f$ for a pure state should be a singular distribution. Note that for mixed states this need not be true — for the quantum canonical ensemble we get in the limit the classical canonical phase density [1],

4) Let A be an observable which possesses classical limit and $A|\Psi\rangle = a|\Psi\rangle$. The real and imaginary parts of the eigenequation give:

$$A(q,p)\cos\left(\frac{\hbar}{2}\Lambda\right)\frac{1}{h} f_\Psi(q,p) = \frac{1}{h} a(\hbar) f_\Psi(q,p),$$

$$A(q,p)\frac{2}{\hbar}\sin\left(\frac{\hbar}{2}\Lambda\right)\frac{1}{h} f_\Psi(q,p) = 0.$$

In the limit $\hbar \to 0$

$$A_{cl}(q, p) f_{lim}(q, p) = (\lim_{\hbar \to 0} a(\hbar)) f_{lim}(q, p),$$

$$\{A_{cl}, f_{lim}\} = 0,$$

here $\{\ ,\ \}$ denotes the Poisson bracket.

If $a_0 = \lim_{\hbar \to 0} a(\hbar)$ exists the first equation tells us that f_{lim} is a distribution with support contained in the set

$$\{(q, p) : A_{cl}(q, p) = a_0\}. \tag{8}$$

For a sufficiently regular function A_{cl} this set consists of isolated points, two-dimensional sets and curves. In the former two cases the second equation vanishes. For curves the Poisson bracket $\{A_{cl}, f_{lim}\}$ is simply the derivative of f_{lim} along the curve. Thus, if the gradient of A_{cl} does not vanish, $f_{lim}(q, p)$ should be constant on the curve (as a distribution). So

$$f_{lim}(q, p) = \sum_j c_j \delta_j (A_{cl}(q, p) - a_0) \tag{9}$$

where δ_j is the Dirac delta function restricted to the j-th connected component of the set (8).

6. *Eigenstates of the Hamiltonian, discrete spectrum, case (a)*

Now we shall show that for the Hamiltonian of the form

$$\boldsymbol{H} = \frac{1}{2m} \boldsymbol{p}^2 + V(\boldsymbol{q}),$$

the limit of an eigenstate from the discrete spectrum is the classical state of rest at the point where $V(q)$ has the absolute minimum.

We shall assume the following properties of $V(q)$:

1) V is differentiable up to the third order,
2) V has only one absolute minimum at the point $q = 0$,
3) $V(0) = 0$ and $V''(0) > 0$,
4) $\liminf_{q \to \pm\infty} V(q) > 0$ but for some N, $V(q)\bar{q}^N$ is bounded for $q \to \pm\infty$.

By means of the substitutions

$$x = \sqrt{\hbar}\, z, \qquad \phi_n(z|\hbar) = \hbar^{1/4} \Psi_n(\sqrt{\hbar}\, z|\hbar), \qquad \varepsilon_n(\hbar) = \frac{1}{\hbar} E_n(\hbar),$$

we transform the equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right) \Psi_n(x|\hbar) = E_n(\hbar) \Psi_n(x|\hbar) \tag{10}$$

into

$$\left(-\frac{1}{2m}\frac{d^2}{dz^2}+\tfrac{1}{2}V''(0)z^2+U(z,\hbar)\right)\phi_n(z,\hbar) = \varepsilon_n(\hbar)\phi_n(z,\hbar). \tag{11}$$

As $\hbar \to 0$, $U(z, \hbar)$ tends to 0 in the strong sense on a dense subspace of $L^2(R)$ (e.g. Schwartz test functions). We shall see that ϕ_n tends to $\phi_n^0(z)$ — the solution of (11) for $U(z, \hbar) = 0$.

From the variational max–min characterization of eigenvalues we obtain $\varepsilon_n(\hbar) \leqslant \varepsilon_n(0)$. Comparing $\varepsilon_n(\hbar)$ with the eigenvalues $\alpha_n(\hbar)$ of (11) with the potential replaced by the following function:

$$\begin{aligned} W(z,\hbar) &= \tfrac{1}{2}V''(0)z^2-C \text{ for } |z| \leqslant \hbar^{-1/8}a, \\ &\tfrac{1}{2}V''(0)\hbar^{-1/4}a^2-C \text{ for } |z| > \hbar^{-1/8}a, \\ C &= \tfrac{1}{3}\hbar^{1/8}a^3 \sup_{(-a,a)} |V'''(x)|, \end{aligned} \tag{12}$$

the choice of a depends on the value of lim inf V, we get $\alpha_n(\hbar) \leqslant \varepsilon_n(\hbar)$. The difference $W(z; \hbar)-\frac{1}{2}V''(0)z^2$ converges to 0 as U does. The values of $\alpha_n(\hbar)$ increase as $\hbar \to 0$ and so $\varepsilon_n(0)$ is a stable point of the spectrum of (11) with (12) (Kato (11], Ch. VIII § 1). Thus $\varepsilon_n(0)$ is also a stable point with respect to $\varepsilon_n(\hbar)$. With the help of theorems on the generalized strong convergence from [11] we conclude that

$$|\phi_n(\hbar)\rangle\langle\phi_n(\hbar)| \underset{\hbar\to 0}{\to} |\phi_n^0\rangle\langle\phi_n^0| \quad \text{(strong limit)}.$$

From (1) we have

$$\frac{1}{h}f_n(q,p|\hbar) = \frac{1}{(2\pi)^2}\int dtdse^{-i(tq+sp)}$$

$$\langle\phi_n|\exp\left(i\sqrt{\hbar}\left(tz-is\frac{\partial}{\partial z}\right)\right)|\phi_n\rangle \to \delta(q)\delta(p) \quad \text{(limit of distributions)}.$$

Generalization to minima of higher order is trivial. The result is in accordance with (9) for $E_n(\hbar) \to 0$ as $\hbar \to 0$.

7. Eigenstates of the Hamiltonian, discrete spectrum, case (b)

We choose a fixed value of energy E in the region of discrete spectrum of (10). To the assumptions 1) and 4) concerning $V(q)$ from the preceding section we add further restrictions that there are only two classical turning points for the energy E and the first derivative of $V(q)$ must not be equal to 0 in the neighbourhoods of the turning points. We may use instead of $\Psi_n(x/\hbar)$ its WKBJ approximant (for detailed evaluations cf. [12]).

In the "classical region" it has the form

$$\Psi_{\mathrm{WKB},n}(x) = a_n(\hbar)\left(\frac{1}{2}\int_{q_1}^{q_2}\frac{dy}{\sqrt{\alpha_n - V(y)}}\right)^{-1/2}\frac{1}{\sqrt[4]{\alpha_n - V(x)}}$$

$$\times\cos\left(\frac{\sqrt{2m}}{\hbar}\int_{q_1}^{x}\sqrt{\alpha_n - V(y)}\,dy + \frac{\pi}{4}\right),$$

where $\underset{i=1,2}{q_i} = q_i(\alpha_n(\hbar))$ are the turning points for the energy $\alpha_n(\hbar)$).

$\alpha_n(\hbar)$ is the smaller value of energy fulfilling the Bohr-Sommerfeld condition and greater than E, $a_n(\hbar)$ is a normalization constant and $a_n \to 1$ as $\hbar \to 0$. Now we calculate the limit of

$$\int \Psi^*_{\mathrm{WKB},n}\left(x - \frac{\hbar u}{2}\right)\Psi_{\mathrm{WKB},n}\left(x + \frac{\hbar u}{2}\right)\varphi(x)dx,$$

φ being a test function, $u \in (u_1, u_2)$.

Let us examine the intervals $(q_1(E)-\varepsilon, q_1(E)+\varepsilon)$ $(q_2(E)-\varepsilon, q_2(E)+\varepsilon)$ and the remaining "classical" and "nonclassical" regions separately. In the "nonclassical" regions the limit is 0 uniformly in u. In the "classical" domain we get due to the Riemann-Lebesgue lemma

$$\left(\frac{1}{2}\int_{q_1(E)}^{q_2(E)}\frac{dy}{\sqrt{E-V(y)}}\right)^{-1}\frac{1}{2}\int_{q_1(E)+\varepsilon}^{q_2(E)-\varepsilon}\frac{\cos(\sqrt{2m}\,u\sqrt{E-V(x)})}{\sqrt{E-V(x)}}\varphi(x)dx$$

also uniformly in u. The contribution from the ε — neighbourhoods is of the order $\sqrt{\varepsilon}$, the evaluation is independent of u_1, u_2. Thus from (1) we obtain

$$f_{\mathrm{lim},E}(q, p) = \frac{1}{\sqrt{2m}}\left(\int_{q_1(E)}^{q_2(E)}\frac{dy}{\sqrt{E-V(y)}}\right)^{-1}\delta(H_{\mathrm{cl}}(q, p) - E),$$

as we should expect from (9).

Similar analysis was performed by Schipper [12], but his conclusions were slightly different.

8. Eigenstates of the Hamiltonian, continuous spectrum

We again use the WKBJ approximation for the wave function. The results differ in the cases of one and no turning points. For the latter case

$$\Psi^{\pm}_{\mathrm{WKB},E}(x) = a(\hbar, E)\sqrt[4]{\frac{m}{2}}\,\frac{\exp\left(\pm\frac{i\sqrt{2m}}{\hbar}\int_0^x\sqrt{E-V(y)}\,dy\right)}{\sqrt[4]{E-V(x)}},$$

with

$$\langle \Psi^{\pm}_{\mathrm{KWB},E} | \Psi^{\pm}_{\mathrm{WKB},E'} \rangle \approx |a|^2 h\delta(E-E') \quad \text{for} \quad E \approx E',$$

so (6)

$$|a| \to 1 \quad \text{for} \quad h \to 0.$$

By similar arguments as in Section 7 we obtain

$$f^{\pm}_{\mathrm{lim},E}(q, p) = \sqrt{\frac{m}{2}} \frac{\delta(p \pm \sqrt{2m(E-V(q))})}{\sqrt{E-V(q)}}.$$

Moreover, we easily check that for $|\Psi\rangle = c_1|\Psi^+\rangle + c_2|\Psi^-\rangle$ we get

$$f_{\mathrm{lim},\Psi} = \sqrt{\frac{m}{2}} \frac{|c_1|^2\delta(p+\sqrt{2m(E-V)}) + |c_2|^2\delta(p-\sqrt{2m(E-V)})}{\sqrt{E-V(q)}}$$

that is the degeneracy of the eigenstate remains in the classical limit, but the interference vanishes.

For one turning point there is no degeneracy and the result is

$$f_{\mathrm{lim},E} = \tfrac{1}{2}\,\delta(H_{\mathrm{cl}}(q, p) - E).$$

9. *The equation of motion*

To complete our considerations let us remind that the quantum equation of motion (5) transforms in the limit into the classical Liouville equation [3].

10. *Concluding remarks*

The main result of our discussion is a manifest confirmation of the view that classical counterparts of quantum states are ensembles of the classical statistical mechanics rather that "states" of "pure" classical mechanics. In particular the limit of quantum eigenstates are "classical eigenstates" — singular probability densities on the phase space confined to sets of constant values of the observable and constant on them. This result is obvious: the "limit state", if exists, must be fully determined by the same set of parameters — quantum numbers — as the quantum state. In spite of this the "pure mechanical" picture of the classical limit seems to be more popular, although the presented above point of view is nearly as old as quantum mechanics itself. It was proposed by Van Vleck [13] in 1928. Van Vleck's considerations based on the approximation of the phase of the wave function by a complete integral of the Hamilton–Jacobi equation (cf. also [14]). Recently Sławianowski [15] discussed the analogies between quantum and classical mechanics using the language of differential geometry and reached the same conclusions.

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