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SOME REMARKS ON THE WIGNER TRANSFORM AND THE WIGNER-POISSON SYSTEM

C. Sean Bohun[1)], Reinhard Illner[2)] and Paul F. Zweifel[3)]

1,2) *Department of Mathematics and Statistics, University of Victoria, P. O. Box 3045, Victoria, B.C., Canada V8W 3P4*

3) *Center for Transport Theory and Statistical Physics, Virginia Polytechnic Institute and State University, Blacksburg, Va. 24061, U.S.A.*

ABSTRACT

We discuss the derivation of the quantum Liouville equation and the Wigner-Poisson system (or quantum Vlasov equation) from elementary quantum mechanical principles via the Wigner transformation.

1. Introduction

In this paper, we use the ideas of Imre, Özimir, Rosenbaum and Zweifel [3] to derive the quantum Liouville equation and to develop the physical basis of the Wigner method. However, we avoid the use of non-normalizable quantum states which mars, to some extent, the discussion of Imre et al. Our treatment is similar to Wigner [10], who defined the Wigner function first and then derived the evolution equation that it obeyed. Markowich [5] began with the evolution equation and proved that a Wigner function constructed from wavefunctions was a solution. While Markowich's treatment is completely rigorous, it does not serve to explicate the physical content of the Wigner function in any detail. Wigner's analysis is more formal - Markowich's work serves to make it mathematically precise. Our treatment is semi-formal, but could be made precise along the lines of Ref. [5], a task we do not undertake here. The reason for our chosen approach is that we feel it provides an excellent intuition into the meaning of the Wigner method and, in particular, it's *raison d'être*. It replaces the heuristic treatment of Ref. [3].

2. The Wigner Transform

Let A represent a (linear) operator in the Hilbert space $\mathcal{H}$ of quantum states; specifically, think of $\mathcal{H} = L^2(\Re^{3N})$ for a system containing N particles. We shall denote the position operator by X and the momentum operator by P; lower case letters x and p simply denote points in $\Re^{3N}$. Also, let $(u_i)_{i=1}^{\infty}$ be an orthonormal basis for $\mathcal{H}$. Then

Definition. The *Wigner transform* $A_w(x,p)$ of an operator $A : \mathcal{H} \to \mathcal{H}$ is

$$A_w(x,p) := \int_{\Re^{3N}} e^{ip\cdot z/\hbar} \sum_{l,k} u_l\left(x - \frac{z}{2}\right) \bar{u}_k\left(x + \frac{z}{2}\right)(u_l, Au_k)\, dz. \tag{1}$$

Here, $\hbar$ is Planck's constant (scaled by 2π) and the inner product (f,g) is assumed to be linear in g (Reed-Simon notation) [9]. An example of a technical question we do not address here is, for what class of operators does the series in (1) converge [2]?

Proposition 1. *For every trace class operator A,*

$$\text{Tr } A = (2\pi\hbar)^{-3N} \int_{\Re^{3N}\times\Re^{3N}} dx\, dp\, A_w(x,p). \tag{2}$$

(*If A is not trace class, the integral is unbounded.*)

Proof. The simple proof is based on the fact that the dp integral of Eq. (1) gives $\delta(z)(2\pi\hbar)^{3N}$ while the dx integral gives δ_{kl}.

One proves similarly

Proposition 2. *Let A, B be trace class operators in $\mathcal{H}$ such that AB is trace class. Then,*

$$\text{Tr } AB = (2\pi\hbar)^{-3N} \int_{\Re^{3N}\times\Re^{3N}} dx\, dp\, A_w(x,p) B_w(x,p). \tag{3}$$

This result is a bit unexpected since when computing traces, there is usually a sum over intermediate states which is not the case in the Wigner representation!

The Wigner *function* $\rho_w(x,p)$, can be defined as the Wigner transform of the density matrix ρ [8]. Since quantum averages, or expectation values, are computed according to

$$\langle A\rangle = \mathrm{Tr}\ \rho A,$$

proposition 2 tells us how to compute such averages by integration over the phase space $\Re^{3N}\times\Re^{3N}$, in analogy with statistical mechanics. The real variables x and p may be thought of as the classical position and momentum variables, as we now explain.

Proposition 3. *Let the operator A be a function of X alone; $A = A(X)$. Then $A_w(x,p) = A(x)$. Similarly if the operator $B = B(P)$, then $B_w(x,p) = B(p)$.*

Proof. Since $A(X)$ is a multiplication operator [8], [4], we can write the inner product in Eq. (1) as

$$(u_l, A(X)u_k) = \int_{\Re^{3N}} \bar{u}_l(y)A(y)u_k(y)\,dy. \tag{4}$$

Now

$$\sum_l u_l\left(x-\frac{z}{2}\right)\int_{\Re^{3N}} \bar{u}_l(y)A(y)u_k(y)\,dy = A\left(x-\frac{z}{2}\right)u_k\left(x-\frac{z}{2}\right),$$

so Eq. (1) can be written as

$$A_w(x,p) = \int_{\Re^{3N}} e^{ip\cdot z/\hbar}\sum_k \bar{u}_k(x\frac{z}{2})u_k\left(x-\frac{z}{2}\right)A\left(x-\frac{z}{2}\right)\,dz.$$

Since, in the sense of Hilbert space,

$$\sum_k \bar{u}_k\left(x-\frac{z}{2}\right)u_k\left(x+\frac{z}{2}\right) = \delta(z)$$

the result follows.

The proof of the second half of the proposition, concerning $B(P)$, is similar, except that one introduces the Fourier integral representation of the basis vectors u_l:

$$\tilde{u}_k(p) = (2\pi\hbar)^{-3N/2} \int e^{-ip\cdot y/\hbar} u_k(y)\, dy \tag{5}$$

and uses the fact that in momentum space [10], $B(P)$ becomes the multiplication operator $B(p)$.

We consider this proposition sufficient justification for viewing the real variables x and p as the classical position and momentum ($3N$) vectors of the system. In the same way, the Wigner transform of the density matrix ρ has some similarity to the classical distribution function of statistical mechanics.

If the wavefunction of a system is indeterminate, it may still be described as the projection sum over the states of the ensemble. Specifically, if the states $\Psi = \{\psi_k\}$ of the ensemble systems are distributed with probilities $\{\lambda_k\}$ then the density operator may be written as [8], [4], [1]

$$\rho = \sum_k \lambda_k P_k$$

where P_k is the orthogonal projection onto the state vector ψ_k. We observe that the ψ_k obey the time-dependent Schrödinger equation

$$i\hbar\partial_t\psi_k = H\psi_k, \quad \psi_k(t=0) = \varphi_k \tag{6}$$

where H is the Hamiltonian of the N-body system. Also $\sum_k \lambda_k = 1$; for a system in a *pure state*, ψ_{k_0} say, $\lambda_k = \delta_{k,k_0}$.

From Eq. (1) we find immediately

$$\rho_w(x,p) = \sum_k \lambda_k \int_{\Re^{3N}} e^{iz\cdot p/\hbar}\, \psi_k\left(x - \frac{z}{2}\right) \bar{\psi}_k\left(x + \frac{z}{2}\right) dz. \tag{7}$$

Except for the sum over k, this is the formula with which Wigner [10] began his treatment. It is also the formula which Markowich [5] derived as a solution of the quantum Liouville equation.

Since Tr $\rho = \sum_k \lambda_k = 1 < \infty$, ρ is trace class. Therefore, using proposition 1, we observe

$$\text{Tr } \rho = 1 \implies \int_{\Re^{3N}\times\Re^{3N}} \rho_w(x,p)\, dx\, dp = (2\pi\hbar)^{3N}.$$

This Wigner function can not be a true distribution, because it is not positive; it is real because ρ is self-adjoint. The Wigner transform of a general operator is not necessarily real [7]. However, the spatial density $n(x)$ is positive

$$\begin{aligned} n(x) &:= (2\pi\hbar)^{-3N} \int_{\Re^{3N}} dp\, \rho_w(x,p) \\ &= \sum_k \lambda_k |\psi_k(x)|^2. \end{aligned} \tag{8}$$

In fact, Eq. (8) is the usual expression for the spatial density in standard quantum mechanics [8]. Similarly, the density in momentum space is readily seen, by integrating ρ_w over x and using Eq. (5), to be

$$\begin{aligned} h(p) &:= (2\pi\hbar)^{-3N} \int_{\Re^{3N}} dx\, \rho_w(x,p) \\ &= \sum_k \lambda_k |(2\pi\hbar)^{-3N/2} \int_{\Re^{3N}} e^{-ip\cdot x/\hbar} \psi_k(x)\, dx|^2 \\ &= \sum_k \lambda_k |\tilde{\psi}_k(p)|^2 \end{aligned} \tag{9}$$

which is also standard. According to proposition 3, if $A = A(X)$ then

$$\langle A \rangle = \int_{\Re^{3N}} A(x) n(x)\, dx \tag{10.a}$$

while if $B = B(P)$

$$\langle B \rangle = \int_{\Re^{3N}} B(p) h(p)\, dp. \tag{10.b}$$

More generally, for any operator C

$$\langle C \rangle = (2\pi\hbar)^{-3N} \int_{\Re^{3N}\times\Re^{3N}} C_w(x,p) \rho_w(x,p)\, dx\, dp. \tag{10.c}$$

3. Quantum Transport Equation

We now derive a kinetic equation for ρ_w assuming that the Hamiltonian H is of the form

$$H = -\sum_{i=1}^{N} \frac{\hbar^2}{2m_i} \Delta_i + V(x). \tag{11}$$

From Eqs. (6) and (7),

$$\begin{aligned} i\hbar\partial_t\rho_w &= -\sum_k \lambda_k \sum_{i=1}^N \frac{\hbar^2}{2m_i} \\ &\times \int_{\Re^{3N}} e^{ip\cdot z/\hbar}\left[\left(\Delta_{x_i-z_i/2}\psi_k^-\right)\bar{\psi}_k^+ - \psi_k^-\left(\Delta_{x_i+z_i/2}\bar{\psi}_k^+\right)\right] dz \\ &+ \sum_k \lambda_k \int_{\Re^{3N}} e^{ip\cdot z/\hbar}\left[V\left(x-\frac{z}{2}\right) - V\left(x+\frac{z}{2}\right)\right]\psi_k^-\bar{\psi}_k^+ \, dz \end{aligned} \tag{12}$$

where $\psi_k^\pm = \psi(x \pm \frac{z}{2})$. The Fourier transform of the Wigner function with respect to momentum is defined by

$$u(x,\eta) = \int e^{-ip\cdot\eta}\rho_w(x,p)\,dp \tag{13.a}$$

with inverse

$$\rho_w(x,p) = (2\pi)^{-3N}\int e^{i\eta\cdot p}u(x,\eta)\,d\eta. \tag{13.b}$$

From Eq. (7) we see that

$$u(x,\eta) = (2\pi\hbar)^{3N}\sum_k \lambda_k\psi_k\left(x-\frac{\hbar\eta}{2}\right)\bar{\psi}_k\left(x+\frac{\hbar\eta}{2}\right). \tag{14}$$

Thus, the second term on the right hand side of Eq. (12) can be written

$$-\Theta(V)\,\rho_w(x,p) \tag{15}$$

where $\Theta(V)$ is the pseudo-differential operator with symbol

$$Sym\ \Theta(V) = V\left(x+\frac{\hbar\eta}{2}\right) - V\left(x-\frac{\hbar\eta}{2}\right). \tag{16}$$

The first term on the right hand side of Eq. (12) can be simplified by partial integration to

$$\begin{aligned} i\hbar & \sum_k \lambda_k \sum_{i=1}^N \frac{2p_i}{m_i}\int_{\Re^{3N}} dz\, e^{ip\cdot z/\hbar}[\bar{\psi}_k^+\nabla_{z_i}\psi_k^- - \psi_k^-\nabla_{z_i}\bar{\psi}_k^+] \\ = & -i\hbar v\cdot\nabla_x\rho_w(x,p) \end{aligned} \tag{17}$$

where we have introduced the velocity vector v with components p_i/m_i. Putting together Eqs. (12), (15) and (17) leads to the quantum Liouville equation

$$\partial_t \rho_w + v \cdot \nabla_x \rho_w - \frac{i}{\hbar}\Theta(V)\rho_w = 0. \tag{18}$$

Therefore, utilizing Eq. (13.a), Fourier transformation of the quantum Liouville equation (18) with respect to v results in

$$\partial_t u + i\nabla_\eta \cdot \nabla_x u - \frac{i}{\hbar}\left[V\left(x + \frac{\hbar\eta}{2}\right) - V\left(x - \frac{\hbar\eta}{2}\right)\right] u = 0 \tag{19.a}$$

which is to be compared to the Fourier transform of the classical Liouville equation [5]

$$\partial_t \hat{f} + i\nabla_\eta \cdot \nabla_x \hat{f} - \nabla_x V i\eta \hat{f} = 0. \tag{19.b}$$

We have denoted the Fourier transform of the classical particle momentum density $f = f(x,p)$ with respect to momentum as $\hat{f}(x,\eta)$. Then, as $\hbar \to 0$, formally

$$\frac{i}{\hbar}\left[V\left(x + \frac{\hbar\eta}{2}\right) - V\left(x - \frac{\hbar\eta}{2}\right)\right] \;\to\; i\eta\nabla_x V$$

and the quantum Liouville equation (18) turns into the classical Liouville equation.

The mean-field counterpart to the quantum Liouville equation (18) is the Wigner-Poisson system

$$\partial_t \rho_w^1 + v \cdot \nabla_x \rho_w^1 - \frac{i}{\hbar}\Theta(V)\rho_w^1 = 0 \tag{20.a}$$

$$V(x) = \int n(y) v(x-y) dy \tag{20.b}$$

where $x \in \Re^3$, $v \in \Re^3$, $n = \int_{\Re^3} \rho_w^1 \, dv$ and ρ_w^1 is the one-particle Wigner distribution function [6]. As discussed for the corresponding Liouville equations, Eq. (20) turns formally into the Vlasov-Poisson system as $\hbar \to 0$. This is completely transparent if the Fourier transforms of the systems are considered. It is, however, an interesting open problem to show that the global classical solutions of the Wigner-Poisson system converge in this limit to the global classical solutions of the Vlasov-Poisson system.

The previous discussion shows clearly how the quantum Liouville equation (and, in the mean field sense, the Wigner-Poisson system) result via Wigner transformation from systems of Schrödinger equations. Under mild and physically reasonable assumptions on the initial value $\rho_w^1(x,p,0)$ of the Wigner-Poisson system, it is possible to reverse this procedure and obtain solutions of Wigner-Poisson by solving a system of coupled Schrödinger equations [5]. Specifically, let $u(x,\eta)$ be the Fourier transform of $\rho_w^1(x,p,0)$. Define the new variables r,s by

$$r = x + \frac{\hbar\eta}{2}, \quad s = x - \frac{\hbar\eta}{2} \tag{21.a}$$

and set

$$z(r,s,0) = (2\pi\hbar)^{-3} u(x(r,s),\eta(r,s)). \tag{21.b}$$

Assume that z is the kernel of a trace class operator with nonnegative real eigenvalues λ_k, then we can expand z is terms of its normalized eigenfunctions φ_k as

$$z(r,s,0) = \sum_k \lambda_k \varphi_k(s)\bar{\varphi}_k(r), \tag{21.c}$$

i.e.

$$u(x,\eta) = (2\pi\hbar)^3 \sum_k \lambda_k \varphi_k\left(x - \frac{\hbar\eta}{2}\right)\bar{\varphi}_k\left(x + \frac{\hbar\eta}{2}\right).$$

Compare this with Eq. (14). A solution $\rho_w^1(x,p,t)$ of Wigner-Poisson can be constructed by solving coupled systems of Schrödinger equations

$$i\hbar\partial_t\psi_k(x,t) = -\frac{\hbar^2}{2m_k}\Delta\psi_k(x,t) + V(x,t)\psi_k(x,t),$$

$$V(x) = \int_{\Re^3} v(x-y)n(y)\,dy,$$

$$n(y) = (2\pi\hbar)^3 \sum_k \lambda_k |\psi_k(y)|^2,$$

and by forming

$$z(r,s,t) = \sum_k \lambda_k \psi_k(s,t)\bar{\psi}_k(r,t)$$

then taking the inverse Fourier transform of

$$u(x,\eta,t) = (2\pi\hbar)^3 \sum_k \lambda_k \psi_k\left(x - \frac{\hbar\eta}{2}\right)\bar{\psi}_k\left(x + \frac{\hbar\eta}{2}\right).$$

See [5] for details. We note that

$$n(x,t) = u(x,0,t) = (2\pi\hbar)^3 z(x,x,t), \tag{22}$$

i.e. the normalization

$$\int_{\Re^3\times\Re^3} \rho_w^1(x,p)\,dp\,dx = 1,$$

implies that

$$\int_{\Re^3} z(x,x,t)\,dx = (2\pi\hbar)^{-3}. \tag{23}$$

REFERENCES

[1] Dicke, R. H., *Introduction to Quantum Mechanics*, Addison-Wesley, Reading, Mass., (1960).

[2] Folland, G. B., *Harmonic Analysis in Phase Space*, Annals of Mathematical Studies, Princeton University Press, Princeton, (1989); considers many of the technical aspects of the Wigner transformation.

[3] Imre, K. Özizmir, E., Rosenbaum, M. and Zweifel, P. F., *Wigner Method in Quantum Statistical Mechanics*, Journal of Mathematical Physics, (5) **8** (1967), 1097-1108.

[4] Liboff, R. L., *Introductory Quantum Mechanics*, Holden-Day, Inc., Oakland, California, 1980.

[5] Markowich, P. A., *On the Equivalence of the Schrödinger and Quantum Liouville Equations*, Mathematical Methods in the Applied Sciences, **11** (1989), 459-469.

[6] Markowich, P. A., Ringhofer, C., and Schneider, *Semiconductor Equations*, Springer-Verlag, (1989); explains the relationship between ρ_w and ρ_w^1.

[7] Narcowich, F. J. and O'Connell, R. F., *Necessary and sufficient conditions for a phase-space function to be a Wigner distribution*, Physical Review A, (1) **34** (1986), 459-469.

[8] von Neumann, J., *Mathematical Foundations of Quantum Mechanics*, Princeton University Press, Princeton, (1955).

[9] Reed, M. and Simon, B., *Methods of Modern Mathematical Physics I: Functional Analysis*, Academic Press, New York, (1972).

[10] Wigner, E., *On the Quantum Correction for Thermodynamic Equilibrium*, Physical Review, **40** (1932), 749-759.