

Quantum Mechanics without Wave Functions

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The phase space formulation of quantum mechanics is based on the use of quasi-distribution functions. This technique was pioneered by Wigner, whose distribution function is perhaps the most commonly used of the large variety that we find discussed in the literature. Here we address the question of how one can obtain distribution functions and hence do quantum mechanics without the use of wave functions.

I. INTRODUCTION

The phase-space formulation of quantum mechanics (PSFQM), which is based on the Weyl ordering⁽¹⁾ and the Wigner distribution function,⁽²⁾ provides a means of analyzing quantum mechanical systems while still employing a phase-space framework.⁽³⁾ It has been used successfully in a number of different fields, e.g., nuclear,⁽⁴⁾ atomic,⁽⁵⁾ molecular⁽⁶⁾ and solid-state physics,^(7,8) scattering processes,⁽⁹⁾ and quantum optics.⁽¹⁰⁾ The basic idea in these applications is to calculate expectation values via phase-space integration rather than through the conventional operator formalism of quantum mechanics. The Wigner-Kirkwood expansion^(2,11) can be used conveniently in the near-classical limit.

The mathematical base of the PSFQM, i.e., the correspondence between quantum mechanical operators and phase-space functions, has been developed thoroughly.⁽¹²⁻¹⁷⁾ Despite the abundance of literature on the PSFQM, the problem of discrete spectrums for various observables, which is certainly a key element of quantum mechanics, has drawn scant attention until recently.⁽¹⁴⁻¹⁷⁾ Moyal⁽¹⁴⁾ has introduced a set of phase-space

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eigenfunctions to formulate the quantization problem. Eigen-equations that correspond to Schrödinger equations have been found for these phase-space functions. We refer to Cohen for a detailed discussion of such equations for a general class of distribution functions.⁽¹⁵⁾ This approach has little advantage over the conventional one, since phase-space functions are, in general, more complicated than the corresponding Schrödinger wave functions. Bayen *et al.*⁽¹⁶⁾ showed that the spectrum of an operator can be easily obtained from its "resolution function," whose expression will be given below. But it has not been explained how the eigenfunctions could be obtained. Variational principles in PSFQM has been discussed by Cohen.⁽¹⁵⁾ Another useful approximation technique, perturbation theory involving small perturbing potentials, has been developed by Dickman and O'Connell^(8,18) for correlation functions and canonical distribution function, but not for eigenstates. These are the motivations that lead to the present discussions.

In Sec. 2, we present initially a brief review of previous work. Next we show that both functions and eigenvalues can be extracted from the Wigner correspondence of a canonical operator, which can be obtained from the corresponding Bloch equation. Perturbation theory of PSFQM will be established in Sec. 3. Finally, we conclude our discussions in Sec. 4.

We shall confine our attention to the one-dimensional case. Generalization to multidimensional situations are straightforward.

2. QUANTIZATION IN PHASE-SPACE

In a 1932 paper, Wigner⁽²⁾ introduced the following distribution function

$$P(q, p) = \frac{1}{2\pi\hbar} \int dy \left\langle q - \frac{y}{2} | \hat{\rho} | q + \frac{y}{2} \right\rangle e^{ipy/\hbar} \quad (1)$$

to represent a system with a density operator $\hat{\rho}$. Integrations are from $-\infty$ to $+\infty$ unless otherwise indicated. This distribution enables us to evaluate the expectation value of any operator \hat{A} through an integration in phase-space:

$$\begin{aligned} \langle \hat{A} \rangle &= \text{Tr}(\hat{\rho} \hat{A}) \\ &= \iint dp dq P(q, p) A(q, p) \end{aligned} \quad (2)$$

if one defines the phase-space function (the Wigner correspondence) by

$$A(q, p) = \int dy \left\langle q - \frac{y}{2} | \hat{A} | q + \frac{y}{2} \right\rangle e^{ipy/\hbar} \quad (3)$$

In the case of a pure state, $\hat{\rho} = |\psi\rangle\langle\psi|$, the Wigner distribution function yields the correct quantum mechanical marginal probability distributions of position and momentum,

$$\int dp P(q, p) = |\psi(q)|^2 \quad (4)$$

$$\int dq P(q, p) = |\phi(p)|^2 \quad (5)$$

where,

$$\psi(q) = \langle q | \psi \rangle \quad (6)$$

and $\phi(p)$ is the wavefunction in the momentum representation:

$$\phi(p) = (2\pi\hbar)^{-1/2} \int dq \psi(q) e^{-ipq/\hbar} \quad (7)$$

The Wigner correspondence of an operator $\hat{F} = \hat{A}\hat{B}$ is⁽¹⁹⁾

$$F(q, p) = A(q, p) XB(q, p) \quad (8)$$

where

$$X = \exp \left[\frac{\hbar}{2i} \left(\frac{\overleftarrow{\partial}}{\partial p} \frac{\overrightarrow{\partial}}{\partial q} - \frac{\overleftarrow{\partial}}{\partial q} \frac{\overrightarrow{\partial}}{\partial p} \right) \right] \quad (9)$$

and the arrows indicate in which direction the derivatives act, or, alternatively,⁽²⁰⁾

$$F(q, p) = A \left(q - \frac{\hbar}{2i}, p + \frac{\hbar}{2i} \frac{\partial}{\partial q} \right) B(q, p) \quad (10)$$

Next we discuss the quantization problem. Here we are interested in Hermite operators, which represent physical observables. Without losing generality, we shall choose to consider a particular quantity, say the Hamiltonian \hat{H} , for the sake of convenience. The following discussion is true for any arbitrary Hermite operator.

Suppose the Hamiltonian of the system \hat{H} has a spectrum $E_0 < E_1 < \dots$ and corresponding eigenstates $|\psi_n\rangle$, i.e.,

$$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle, \quad n = 0, 1, \dots \quad (11)$$

One asks the question: What is the phase-space correspondence of the Schrödinger equation (11)?

A direct approach to this problem would be the following. Multiplying both sides of (11) by $\langle \psi_n |$ one obtains

$$\hat{H}\hat{\rho}_n = E_n\hat{\rho}_n \quad (12)$$

where

$$\hat{\rho}_n = |\psi_n\rangle\langle\psi_n| \quad (13)$$

is the projector operator to the n th state. One then uses (10) to transform (12) into phase-space language:

$$H(q, p)XP_n(q, p) = E_nP_n(q, p) \quad (14)$$

or

$$H\left(q - \frac{\hbar}{2i} \frac{\partial}{\partial p}, p + \frac{\hbar}{2i} \frac{\partial}{\partial q}\right)P_n(q, p) = E_nP_n(q, p) \quad (15)$$

where $P_n(q, p)$ is the Wigner distribution function for the n th eigenstate. The orthogonality and completeness of $|\psi_n\rangle$, i.e.,

$$\hat{\rho}_n\hat{\rho}_m = \delta_{nm}\hat{\rho}_n \quad (16a)$$

and

$$\sum_n \hat{\rho}_n = 1 \quad (16b)$$

give the following properties, respectively, for its corresponding $P_n(q, p)$:

$$P_n(q, p)XP_m(q, p) = \frac{1}{2\pi\hbar} \delta_{nm}P_n(q, p) \quad (17a)$$

and

$$\sum_n P_n(q, p) = \frac{1}{2\pi\hbar} \quad (17b)$$

Do (17a) and (17b) mean that $P_n(q, p)$ is an orthogonal and complete set in phase-space? The answer is no. It can be seen clearly through the following argument. An arbitrary operator \hat{A} can be expanded by

$$\begin{aligned} \hat{A} &= \left(\sum_n \hat{\rho}_n\right)\hat{A}\left(\sum_m \hat{\rho}_m\right) \\ &= \sum_{n,m} A_{nm}\hat{\rho}_{nm} \end{aligned} \quad (18a)$$

where

$$\hat{p}_{nm} = |\psi_m\rangle\langle\psi_n| \quad (18b)$$

and

$$A_{nm} = \langle\psi_m|\hat{A}|\psi_n\rangle \quad (18c)$$

The phase space transforms of (18a) reads:

$$A(q, p) = (2\pi\hbar) \sum_{n,m} A_{nm} P_{nm}(q, p) \quad (19a)$$

where

$$P_{nm}(q, p) = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dy \psi_n^* \left(q - \frac{y}{2} \right) \psi_m \left(q + \frac{y}{2} \right) e^{ipy/\hbar} \quad (19b)$$

is a set of phase space wave functions first introduced by Moyal.⁽¹⁴⁾ The matrix elements in Eq. (18c) can now be rewritten as follows:

$$\langle\psi_m|\hat{A}|\psi_n\rangle = \iint A(q, p) P_{nm}^*(q, p) dq dp \quad (19c)$$

Hence (19a) is simply the expansion of an arbitrary function $A(q, p)$ on $P_{nm}(q, p)$. In fact the completeness and the orthogonality of Moyal's functions can be easily proven from the definition (19b):

$$\sum_{n,m} P_{nm}^*(q, p) P_{nm}(q', p') = \frac{1}{2\pi\hbar} \delta(q - q') \delta(p - p') \quad (20)$$

Therefore $P_n(q, p)$, which belongs to a subset of Moyal's functions, does not form a complete set in phase-space.

Following the same method used in the derivation of (15), one obtains

$$H \left(q - \frac{\hbar}{2i} \frac{\partial}{\partial p}, p + \frac{\hbar}{2i} \frac{\partial}{\partial q} \right) P_{nm}(q, p) = E_n P_{nm}(q, p) \quad (21)$$

which is Moyal's equation.⁽¹⁴⁾

It is apparent that (15) is just a special case of (21), since $P_{nn}(q, p) = P_n(q, p)$ by definition. We observe that there is no need to consider (21), because if (15) can be solved, eigen wave-functions can be extracted from the distribution function. By using (4), we obtain, apart from an arbitrary phase factor,

$$\psi_n(q) = \left[\int P_n(q, p) dp \right]^{1/2} \quad (22)$$

Compared with the conventional Schrödinger equation, (15) is more complicated and has no practical advantage.

We will now present a new approach to the quantization problem. Consider the unnormalized density operator of a canonical ensemble at temperature T :

$$\begin{aligned}\hat{\Omega} &= e^{-\beta\hat{H}} \\ &= \sum_n e^{-\beta E_n} \hat{P}_n\end{aligned}\quad (23)$$

where $\beta = 1/kT$ and k is the Boltzmann's constant. The Wigner correspondence of (23) is

$$\Omega(q, p, \beta) = (2\pi\hbar) \sum_n e^{-\beta E_n} P_n(q, p) \quad (24)$$

If one defines the Laplace transform of $\Omega(q, p, \beta)$:

$$R(q, p; E) = \int_0^\infty d\beta \Omega(q, p; \beta) e^{-\beta E} \quad (25)$$

by (24) one has

$$R(q, p; E) = \sum_n \frac{2\pi\hbar}{(E + E_n)} P_n(q, p) \quad (26)$$

Hence the spectrum $\{E_0, E_1, \dots\}$ can be obtained as the negatives of the singularities of the Laplace transform of the Wigner phase-space function corresponding to the unnormalized density operator.⁽²¹⁾

As we have seen, this approach to the quantization problem avoids the difficult eigenvalue differential equation problem in the conventional treatment. But there still remains the question of how to obtain eigen wavefunctions in this approach. With that in mind, we turn to the question of the general method of calculating the phase-space function $\Omega(q, p; \beta)$. Now $\Omega(q, p; \beta)$ satisfies the Wigner correspondence of the Bloch equation:^(22-24,3)

$$\frac{\partial \Omega(q, p; \beta)}{\partial \beta} = -H(q, p) \cos \left[\frac{\hbar}{2} \left(\frac{\partial}{\partial q} \frac{\partial}{\partial p} - \frac{\partial}{\partial p} \frac{\partial}{\partial q} \right) \right] \Omega(q, p; \beta) \quad (27)$$

In principle $\Omega(q, p; \beta)$ can be solved from (29) with the initial condition:

$$\Omega(q, p; 0) = 1 \quad (28)$$

If

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q}) \quad (29)$$

its Wigner correspondence is simply

$$H(q, p) = \frac{p^2}{2m} + V(q) \quad (30)$$

and then (29) can be simplified further:⁽²⁴⁾

$$\frac{\partial \Omega(q, p; \beta)}{\partial \beta} = \left[-H(q, p) + 2 \sin^2 \left(\frac{\hbar}{4} \frac{\partial}{\partial q} \frac{\partial}{\partial p} \right) V(q) + \frac{\hbar^2}{8m} \frac{\partial^2}{\partial q^2} \right] \Omega(q, p; \beta) \quad (31)$$

where the $\partial/\partial q$ term in the sine term is to be understood as operating only on $V(q)$.

Once we have obtained $\Omega(q, p; \beta)$, we can calculate the distribution functions for the eigenstates as the following. First of all, we use (25) to obtain the resolvent function and it is clear from (26) that we determine the spectrum E_n from the singularities of the resolvent function. Secondly, we have

$$P_n(q, p) = (2\pi\hbar)^{-1} \lim_{E \rightarrow -E_n} (E - E_n) R(q, p; E) \quad (32)$$

which follows immediately from (26). The eigen wave-function can be obtained through (22).

To make this procedure more clear we consider the one-dimensional harmonic oscillator as an explicit example, the exact solution of (31) in this case being^(1,25)

$$\Omega(q, p; \beta) = \operatorname{sech} \left(\frac{\hbar\omega\beta}{2} \right) \exp \left[-\frac{2}{\hbar\omega} \tanh \left(\frac{\hbar\omega\beta}{2} \right) H(q, p) \right] \quad (33)$$

where

$$H(q, p) = p^2/2m + m\omega^2 q^2/2 \quad (34)$$

The function $R(q, p; E)$ can readily be calculated from the definition (25):

$$R(q, p; E) = \sum_{n=0}^{\infty} 2(-1)^n e^{-2nH/\hbar\omega} L_n(4H/\hbar\omega)^j (E - (n + \frac{1}{2})\hbar\omega) \quad (35)$$

where L_n is the n th Laguerre polynomial. The negatives of singularities of $R(q, p; E)$ give the spectrum

$$E_n = (n + \frac{1}{2})\hbar\omega \quad (36)$$

while (32) gives the distribution function

$$P_n(q, p) = (\pi\hbar)^{-1} (-1)^n e^{-2H/\hbar\omega} L_n(4H/\hbar\omega) \quad (37)$$

The n th eigen wave function is then obtained from (22) and (37):

$$\psi_n(q) = \left(\frac{\alpha^2}{\pi}\right)^{1/4} \left(\frac{1}{2^n n!}\right)^{1/2} e^{-\alpha^2 q^2/2} H_n(\alpha q) \quad (38)$$

where $\alpha = (m\omega/\hbar)^{1/2}$. Eq. (37) is a well-known result but here we have obtained it without prior knowledge of the wave function $\psi_n(q)$.

3. PERTURBATION THEORY IN THE PSFQM

Perturbation expansions have been developed recently by Dickman and O'Connell^{18,19} for the Wigner correspondence of the canonical density operator and the correlation function. In the light of the discussions in Sec. 2, we can formulate the perturbation theory for eigenstates in the PSFQM. We confine our attention to the first-order result but generalization to higher orders is straightforward.

We denote the Wigner correspondence of the perturbed Hamiltonian, eigenvalue and eigen distribution function by

$$H = H_0 + \lambda H_1, \quad E_n = E_n^{(0)} + \lambda E_n^{(1)} \quad (39)$$

and

$$P_n(q, p) = P_n^{(0)}(q, p) + \lambda P_n^{(1)}(q, p) \quad (40)$$

respectively, where λ is the expansion parameter.

Our starting point is (14), which to first order may be written as

$$(H_0 - E_n^{(0)}) X P_n^{(1)} = (E_n^{(1)} - H_1) X P_n^{(0)} \quad (41)$$

Let $P_n^{(0)} X$ act from the left side of both sides of (41), to obtain the lowest order energy shift:

$$E_n^{(1)} = \iint dq dp H_1 P_n^{(0)} \quad (42)$$

To obtain (42) we have used the fact that

$$\hat{\rho}_n \hat{H}_1 \hat{\rho}_n = \langle \psi_n | \hat{H}_1 | \psi_n \rangle \hat{\rho}_n \quad (43a)$$

or,

$$P_n^{(0)} X(H, X P_n^{(0)}) = \left(\iint dq dp H, P_n^{(0)} \right) P_n^{(0)} \quad (43b)$$

Expanding $P_n^{(1)}$ onto Moyal's functions defined in (19b), we have

$$P_n^{(1)}(q, p) = \sum_{\mu\nu} C_{\mu\nu} P_{\mu\nu}^{(0)}(q, p) \quad (44)$$

where $C_{\mu\nu}$ is to be determined.

We then substitute (44) into (41). Using the orthogonality of the Moyal functions, we obtain

$$C_{\mu\nu} = \iint dq dp P_n^{(0)} H, P_n^{(1)} / (E_n^{(0)} - E_\nu^{(0)}), \quad \nu \neq n \quad (45)$$

In the derivation of (45), we have taken advantage of the fact that an arbitrary term linear in $P_{\mu\nu}^{(0)}$ can be added to $P_n^{(1)}$ without any effect on (41). We have chosen

$$C_{\mu n} = 0 \quad (46)$$

so that

$$\iint P_n^{(1)} P_n^{(0)} dq dp = 0 \quad (47)$$

Eqs. (2), (44), (45) and (46) are the desired first order perturbation expansion in the PSFQM.

4. CONCLUSION

We have discussed the quantization problem and perturbation theory in PSFQM. We showed how both eigenvalues and eigen wave-functions can be extracted from the Wigner correspondence of the density operator of a canonical ensemble, which can be obtained from the Wigner correspondence of the Bloch equation.

We have confined our attention to the Wigner version of the PSFQM, which corresponds to Weyl's rule for assigning a quantum mechanical operator to a classical function. Generalization of the present investigation to an arbitrary representation of PSFQM can be worked out starting with the results given by Cohen.⁽¹⁵⁾

From a more general point of view, this paper can be viewed as a small part of the large mosaic of research on the relationship between classical and quantum theories, some of the more prominent parts of the mosaic having been weaved by Professor David Bohm. In particular, we mention a contribution of Bohm and Hiley,⁽²⁶⁾ which is related to our present considerations in the they also start with the work of Wigner and Moyal but—in characteristic style—they approach it from a different point of view. Bohm and Hiley also regard the density matrix as fundamental and treat the wave function as an abstraction. However, they depart from the usual point of view by consideration of a non-Hermitian generalization of the density matrix and, concomitantly, a more generalized phase space. But that is another story.

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