Wigner's Function and Other Distribution Functions in Mock Phase Spaces

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Markov: "In my opinion the various notions can be defined not so much by words which may require additional explanations but by our attitude towards them which is then gradually clarified" (Calculus of Probabilities, 1924, p.2)
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Abstract

This review deals with the methods of associating functions with quantum mechanical operators in such a manner that these functions should furnish conveniently semiclassical approximations. We present a unified treatment of methods and results which usually appear under the expressions Wigner's function, Weyl's association, Kirkwood's expansion, Glauber's coherent state representation, etc.; we also construct some new associations.

Section 1 gives the motivation by discussing the Thomas-Fermi theory of an atom with this end in view.

Section 2 introduces new operators which resemble Dirac delta functions with operator arguments, the operators being the momenta and coordinates. Reasons are given as to why this should be useful. Next we introduce the notion of an operator basis, and discuss the possibility and usefulness of writing an operator as a linear combination of the basis operators. The coefficients in the linear combination are c-numbers and are the c-numbers associated with the operator (in that particular basis). The delta function type operators introduced before can be used as a basis for the dynamical operators, and the c-numbers obtained in this manner turn out to be the c-number functions used by Wigner, Weyl, Kirkwood, Glauber, etc. New bases and associations can now be invented at will. One such new basis is presented and discussed. The reasons and motivations for choosing different bases is then explained.

The copious and seemingly random mathematical relations between these functions are then nothing else but the relations between the expansion coefficients engendered by the relations between the
different bases. These are shown and discussed in this light. A brief
discussion is then given to possible transformations of the $p,q$
labels.

Section 3 gives examples of how the semiclassical expansions are
generated for these functions and exhibits their equivalence.

The mathematical paraphernalia are collected in the appendices.
1. Introduction

In this article we intend to do two things. First, we want to order and summarize the complex of problems and methods which make use of a mock phase-space in quantum mechanics, associated originally with the names of Weyl, Wigner and Moyal, and particularly well adapted to asymptotic expansions in Planck's constant. There is a great proliferation of results and techniques which are related to each other, and whose raison d'être is not always transparent. Often, it is not easy to see the underlying motivation, and to distinguish between necessity and convenience. We hope that we give sufficient intuitive ideas to make the reader sense the reason for the mathematical choice, or steps taken.

Second, we want to show how these methods can be applied in practice. From the abundant literature we chose a particular class of problems, the analysis of stationary states and the associated spectrum for one particle systems. This finds its uses in nuclear physics, and it is in this field that some of the more recent applications have taken place. We do not deal with time-dependent problems, or scattering problems although they, too, are of real interest, in particular in molecular scattering and heavy ion collisions. The scattering problem has been reviewed in a recent paper by Carruthers and Zachariasen 1983, which also has an extensive list of references. Our choice is eclectic, and the literature survey incomplete. We aimed to review the basic intuitive ideas more than the literature. The spirit of the discussion is that of a text to study, and less that of a reference. We beg authors to forgive us when their work is not given sufficient credit.
1.1 The Thomas-Fermi theory

To motivate our use of Wigner's function and semiclassical approximations we discuss here the Thomas-Fermi theory in a manner which brings to the fore the problem-setting and the mathematical quantities to be introduced. Thomas (1926) and Fermi (1927) suggested an ingenious method to describe an atom considering it as a nucleus surrounded by an inhomogeneous atmosphere of electrons. The electrons interact with each other and with the nucleus through Coulomb forces while at the same time they also satisfy the exclusion principle. The model bears a close resemblance to Debye's theory of electrolytes, although this analogy has not been used by Thomas or Fermi. In the electrolyte theory the thermal agitation acts as a counterbalance to the Coulomb attraction, while here the statistical repulsion embodied in the exclusion principle has this role. Both Thomas and Fermi now make strong use of (semi) classical arguments. To stress this we will rephrase them so as to exhibit the main assumptions explicitly.

The two basic quantities used to describe a classical gas interacting through pair interactions are the singlet distribution function $f_1(p,q)$ and the pair distribution $f_2(p_1,q_1;p_2,q_2)$. Usually, (but not always) they are normalised as

$$\int f_1(p,q)d^3pd^3q = N,$$

$$\int f_2(p,q;p',q')d^3pd^3q' = (N-1)f_1(p,q).$$

The singlet distribution function is usually displayed in the six-dimensional $\mu$-space, and specifies the number of particles with coordinates $q$ and momenta $p$ in the small volume element $d^3pd^3q$. The pair distribution function specifies the number of particles at $q_1$ with $p_1$ and the number of particles at $q_2$ with $p_2$ in the volume elements.
\[ d^3p_1d^2q_1, d^3p_2d^3q_2. \] Given this, the total energy of the system can immediately be written down as

\[ E = \int \left( \frac{1}{2m} p^2 V(q) \right) f_1(p, q)d^3p_1d^3q_1 + \frac{1}{2} \int d^3p_1d^3q_1 d^3p_2d^3q_2 u(q, q') f_2(p, q; p', q') \]

where \( V(q) \) is the external potential, and \( u(q, q') \) is the pair potential acting between particles located at points \( q \) and \( q' \).

The object is to determine this energy. To do this one makes two assumptions. First, one approximates \( f_2 \) as being proportional to the product of the singlet distribution function

\[ f_2(p, q; p', q') = \frac{f_1(p, q)}{N(N-1)} \cdot \frac{f_1(p', q')}{N} \]

The \((1-1/N)\) factor is needed to give the correct normalization. (In the early literature the \(1/N\) part has been called the Fermi-Amaldi correction.)

Second, we assume that the exclusion principle can be incorporated by assuming that \( f_1 \) can take only two values \( 1/h^3, 0 \) for each spin species, or \( 2/h^3, 0 \) if we do not distinguish the spin-up and spin-down electrons. Thus \( f_1 \) can be viewed as describing a homogeneous, incompressible fluid in the \( u \)-space.

The second assumption is thus based on the belief that the exclusion principle states that only one phase point per spin species can occupy a \( u \)-space cell of size \( h^3 \). This, of course, must be taken with a grain of salt since the variables \( p \) and \( q \), as momenta and coordinates cannot be specified simultaneously in quantum mechanics. Nor is it likely that the exclusion principle can be stated in terms of the singlet particle distribution alone, since this principle is a symmetry condition which involves the configuration of any two particles.
Accepting then these assumptions, \( f_1 \) (and hence also \( f_2 \)) is completely specified if we give in the \( \mu \)-space the 5 dimensional surfaces on which \( f_1 \) exhibits discontinuities. If we seek the ground state of the system it is likely that there is only one such hypersurface separating the filled-in region from the rest of the \( \mu \)-space. Let this hypersurface have the equation \( g(p,q) = 0 \). The hypersurface is determined by the condition that the ground state energy is minimum, hence its variation must vanish, given that the variation does not alter the number of particles, the incompressibility condition imposed on \( f_1 \), and the value of the entropy, which is zero in this case. Both the incompressibility condition and the entropy condition is satisfied if we vary \( f_1 \) by varying the surface \( g \) only. Performing the variation we get the usual Thomas-Fermi theory expressed in terms of \( f_1(p,q) \), and \( f_2(p_1q_1,p_2q_2) \). (See Appendix II, Eqs. AII.1 to 1.4.) The problem we face now is the adaptation of this argument to quantum mechanics. The functions \( f_1(p,q), f_2(p,q;p',q') \) do not exist, and we must find the quantum-mechanical equivalent.

Summary: The classical one body distribution function \( f(p,q,t) \) gives the probability that a particle has the coordinates around \( q \) and the momenta around \( p \), at time \( t \); it can be used to find average values of dynamical quantities \( A(p,q) \). The success of the Thomas-Fermi theory suggests that a similar quantity should also be useful in a quantum-mechanical system.

2. The Weyl correspondence, Wigner's function and their generalisations

What happens if we wish to cast this formalism in terms of quantum mechanics? The basic problem is, of course, that \( f(p,q) \) no longer
exists since \( q \) and \( p \) cannot be measured simultaneously. What quantity should replace it? We shall consider a one-particle system in three dimensions. It is easy to generalize this if needed. (By pure insight P.A.M. Dirac 1930 and W. Heisenberg 1931 introduced a quantity \( f(p,q) \) identical to Wigner's function form which they constructed the density matrix in the \( x \) representation.)

2.1. Probability distributions and characteristic functions

The state of the system is described by the density operator \( \hat{\rho} \). Then, the probability that in an observation the position will have the value \( q' \) is given by \( \text{Pr}(q') = \text{Tr}(\delta(q-q')\hat{\rho}) \); the probability that the momentum will be observed to have the value \( p' \) is \( \text{Pr}(p') = \text{Tr}(\delta(p-p')\hat{\rho}) \).

This gives the conventional result \( \text{Pr}(p') = <p'|\hat{\rho}|p'> \). First, it is easy to verify that if \( |p'\rangle\langle p'| \) is the projection operator to the eigenstate \( |p'\rangle \) of \( \hat{p} \) associated with the eigenvalue \( p' \) then \( \delta(p-p') = |p'\rangle\langle p'| \) since both sides give the same matrix elements. But \( \text{Tr}(|p'\rangle\langle p'|\hat{\rho}) = <p'|\hat{\rho}|p'> \). In general the probability that the observable \( \hat{u} \) will be observed to have the value \( u' \) is given by \( \text{Pr}(u') = \text{Tr}(\delta(u-u')\hat{\rho}) \), if \( \hat{u} \) has a continuous spectrum. We may also evaluate \( \text{Tr}(\delta(p-p')\delta(q-q')\hat{\rho}) \), or \( \text{Tr}(\delta(q-q')\delta(p-p')\hat{\rho}) \), and consider this quantity as the analogue of \( f(p',q') \). These quantities, however, are not the same, are not symmetrical in \( \hat{p} \) and \( \hat{q} \) and are not positive everywhere. Furthermore, they will be complex. In spite of these shortcomings either of these quantities may be used as analogues of \( f(p,q) \). We shall discuss them under the name of Kirkwood's association. However, first we proceed to find a more symmetrical quantity which has the advantage of being real. In order to do this conveniently we will consider not only the "probability" distributions but also
their Fourier transforms and the characteristic functions associated with them. This way we construct Table 2.1. In this Table we have introduced a sequence of dimensionless $\hat{A}$ operators which all qualify to generate quantities which can be used to compute expectation values, and are analogous to the classical $f(p,q)$. The operators $\hat{A}_k^+, \hat{A}_k^-$ are proportional to products of $\delta$ functions with operator arguments, while in the Fourier transform definitions they carry phase factors. $\hat{A}$ is a new type of delta operator function which is obtained in the Fourier transform definition using the $\hat{T}$ operators (which do not change if we exchange $p$ and $q$!) and no extra factors. This expression is not the symmetrized product of $\delta(\hat{p}-p)$ and $\delta(\hat{q}-q)$, i.e. $\hat{A}^+(\hat{A}_k^+ + \hat{A}_k^-)/2$, since the latter acquires the factor $\cos \left(\frac{\pi uv}{2}\right)$ in the Fourier transform definition. Finally we have introduced in general $\hat{A}(p',q')$ in which a function $F(u,v)$ appears in the Fourier transform definition. We note that a Fourier transform of a product leads to a convolution of the objects associated with the individual Fourier transforms. Thus $\hat{A}(p',q') = \int dp dq \hat{A}(p,q) F(p-p',q-q')$. The $\hbar^3$ factors were introduced to make the $\hat{A}$ operators dimensionless. Similarly the functions $f(p,q) = Pr(p,q)/(2\pi\hbar)^3$ are also dimensionless.

The surfeit of $\hat{A}$ operators has its origin in the physical fact that $\hat{p}$ and $\hat{q}$ cannot be simultaneously observed, hence no Hermitian operator $\hat{\omega}(p,q)$ exists which could be used to specify a probability distribution through the rule $\text{Tr}(\hat{\omega}\hat{\rho})$.

As we shall soon see, the different $f$ functions eg. $f_{\text{H}}$, $f_{\text{K}}^+$, $f_{\text{K}}^-$, share many useful properties with the classical $f$ function. However, they are not proper probability densities because they are not positive definite, and $f_{\text{K}}^+$, $f_{\text{K}}^-$ are not even real.
A necessary condition for the usefulness of the different $f$ functions is that from any one of them we should be able to recover $\hat{\rho}$.

(Different $A$ operators were studied, among others, by L. Cohen 1966, G.S. Agarwal and E. Wolf 1970a. Kirkwood 1933 describes an approximation scheme which can be recast in an equivalent form using the $\hat{A}_N^k$ operators.)

Summary: Classically $f(p', q', t)$ can be written as the average value of the dynamical quantity $\delta(p - p') \delta(q - q')$ where $p', q'$ are particular values of the dynamical quantities $p$ and $q$. We then expect that in a quantum mechanical description the averages of the dynamical operator $\delta(\hat{p} - p') \delta(\hat{q} - q')$ will play an important role. When averaged with respect to the density operator $\rho$ we should obtain a function similar to the classical $f(p, q, t)$. Because the operators $\delta(\hat{p} - p')$ and $\delta(\hat{q} - q')$ do not commute, there are many combinations of these two operator functions such as $\hat{A}, \hat{A}_N = \hat{A}_K \hat{A}_N, \hat{A}_K$ etc., which qualify to produce such a function upon averaging.
Table 2.1

\[ \Pr(p') = \text{Tr}\left(\delta(\hat{p}-p')\rho\right) \]
\[ \Pr(q') = \text{Tr}\left(\delta(\hat{q}-q')\rho\right) \]
\[ \Pr_k^{+}(p',q') = \text{Tr}\left(\delta(\hat{p}-p')\delta(\hat{q}-q')\beta\right) \]
\[ = \text{Tr}\left(\frac{\hat{k}^+}{(2\pi\hbar)^3}\beta\right) \]
\[ \Pr_k^{-}(p',q') = \text{Tr}\left(\delta(\hat{q}-q')\delta(\hat{p}-p')\beta\right) \]
\[ = \text{Tr}\left(\frac{\hat{k}^-}{(2\pi\hbar)^3}\beta\right) \]
\[ \Pr_u(p',q') = \text{Tr}\left(\delta(\hat{q}-q')\delta(\hat{p}-p')\beta\right) \]
\[ = \text{Tr}\left(\frac{\hat{u}}{(2\pi\hbar)^3}\beta\right) \]

\[ \Delta_k(p',q') = \frac{\hbar^3}{(2\pi)^3/2} e^{1+i[u*(\hat{p}-p')+v*(\hat{q}-q')]} d^{3} u d^{3} v \]
\[ \Delta_k^{+}(p',q') = (2\pi\hbar)^3 \delta(\hat{p}-p') \delta(\hat{q}-q') \]
\[ = \frac{\hbar^3}{(2\pi)^3/2} e^{1+i[u*(\hat{p}-p')+v*(\hat{q}-q')]} e^{i\hbar(u+v)/2} d^{3} u d^{3} v \]
\[ \Delta_k^{-}(p',q') = (2\pi\hbar)^3 \delta(\hat{q}-q') \delta(\hat{p}-p') \]
\[ = \frac{\hbar^3}{(2\pi)^3/2} e^{1+i[u*(\hat{p}-p')+v*(\hat{q}-q')]} e^{-i\hbar(u+v)/2} d^{3} u d^{3} v \]
\[ \Delta_F(p,q) \]
\[ = \frac{\hbar^3}{(2\pi)^3/2} e^{1+i[u*(\hat{p}-p')+v*(\hat{q}-q')]} \tilde{F}(u,v) d^{3} u d^{3} v \]

\[ \bar{\Pr}(u) = \int \Pr(p') e^{iu*p'} d^{3} p' = \text{Tr}(e^{iu*p}\beta) \]
\[ \bar{\Pr}(v) = \int \Pr(q') e^{iv*q'} d^{3} q' = \text{Tr}(e^{iv*q}\beta) \]
\[ \bar{\Pr}_k^{+}(u,v) = \text{Tr}(e^{iu*p} e^{iv*q}\beta) \]
\[ = \text{Tr}(e^{i(u+p+v)\beta} e^{i\hbar(u+v)/2}) \]
\[ \bar{\Pr}_k^{-}(u,v) = \text{Tr}(e^{iv*q} e^{iu*p}\beta) \]
\[ = \text{Tr}(e^{i(u+p+v)\beta} e^{-i\hbar(u+v)/2}) \]
\[ \bar{\Pr}_u(u,v) = \text{Tr}(e^{i(u+p+v)\beta}) \]
\[ = \text{Tr}(\beta) \]
\[ \tilde{F}(u,v) = e^{1+i(u*p+v*q)} \]
\[ \tilde{F}_k^{+}(u,v) = e^{1+i(u*p+v*q)} e^{i\hbar(u+v)/2} \]
\[ \tilde{F}_k^{-}(u,v) = e^{1+i(u*p+v*q)} e^{-i\hbar(u+v)/2} \]
\[ \tilde{F}_F(u,v) = e^{1+i(u*p+v*q)} \tilde{F}(u,v) \]
2.2 The Introduction of Basis Operators

Although these constructions were motivated by the density operator, they generalize to an arbitrary operator. We may evaluate the trace of any operator with $\hat{T}$ or $\hat{A}$ to obtain a function. These functions are equivalent to the operators in question since given the function we can reconstruct the operator, and given the operator we can reconstruct the function. (We shall leave aside the beautiful mathematical problem to characterize the class of operators for which this can be done. See, however, Segal 1963, Kastler 1965, Pool 1966 in a different context.) Such an association was first conceived by Weyl in 1928 using the $\hat{T}$ operator, and later, for the density operator, by Wigner using the $\hat{A}$ operator. We shall call both the W association; $\text{Tr}(\hat{A} \hat{P})$ is conventionally called Wigner's function.

However, we can go further, noticing the following. Consider all operators in quantum mechanics, i.e. all operator functions of $\hat{P}$ and $\hat{Q}$. We may multiply them with scalars and we may add them together. Thus, they form a linear vector space, in which the points now are operators. If this be the case, we may ask what is a suitable complete basis in this vector space? Given such a basis, we may write any operator as a linear combination of the basis, the coefficients being complex numbers. The previous considerations amounted to a special selection of basis, the $\hat{T}$ basis or the $\hat{A}$ basis. The expansion coefficients are the complex numbers associated with the operators. Thus we have a very general scheme and the W associations correspond to special choices of bases, the $\hat{T}$ basis or the $\hat{A}$ basis. The $\hat{T}$ basis generates functions in a $u,v$ space, while the $\hat{A}$ basis generates functions in a $p,q$ space which is the dual of the $u,v$ space. The $p,q$ space is in many respects
similar to the phase space, but it is not invariant under canonical transformations, only under linear inhomogeneous transformations. We shall call it the W space. The u,v space is invariant under linear homogeneous transformations, thus it has a preferred origin, or center. Because of this, its geometry is different from the W space.

There is nothing unique about choosing different bases in our operator space, and hence associating different functions with the same operator. Once certain general conditions are satisfied, it is mainly convenience which will determine our choice, reflecting ease of computability, presence of symmetry, etc. From this point of view the different \( T \) and \( \hat{A} \) operators are different choices of bases.

Consider, then a basis \( \hat{B}(\hat{p},\hat{q};a,b) = \hat{B}(a,b) \) (all bases always depend on \( \hat{p},\hat{q} \); hence we cease to indicate explicitly this dependence.) The basis is enumerated by the variables \( a,b \); \( a \) and \( b \) can be continuous or discrete. If we were to deal with a finite dimensional space it would be the latter. We shall write our expressions for \( a,b \) being continuous.

Then

\[
\hat{u} = \int \text{d}a\text{d}b \hat{B}(a,b) \hat{B}(a,b) ,
\]  

(2.1)

and the expansion in coefficients \( \hat{u} \) are the associated functions, or the image of \( \hat{u} \) (with respect to the basis \( B \)).

In order that the basis should be usable \( \hat{B} \) should have an inverse \( \hat{B}^{-1}(a,b) \), in the sense that

\[
\text{Tr}(\hat{B}^{-1}(a,b)\hat{B}(a',b')) = \delta(a-a')\delta(b-b') .
\]

(2.2)

The order under the trace is arbitrary. \( \hat{B}^{-1}(a,b) \) should be carefully distinguished from the reciprocal of \( B \), defined by

\[
\hat{B}^{-1} = \hat{B}^* \hat{B}^{-1} = \hat{1} .
\]

(2.3)
If this be the case two useful relations follow
\[ \tilde{\mathcal{B}}_B^{(a,b)} = \text{Tr}(\mathcal{B}_B^{-(a,b)}) \] (2.4)
\[ \tilde{\mathcal{C}}_B^{(a,b)} = \text{Tr}(\mathcal{C}_B^{(a,b)}) \] (2.5)
(Notice the arrangement of ± signs.) Given two operators \( \hat{A}, \hat{C} \) we find
\[ \text{Tr}(\hat{A}\hat{C}) = \int \text{dadb} \tilde{\mathcal{B}}_B^{(a,b)} \tilde{\mathcal{C}}_B^{-(a,b)} \] (2.6)
Thus, actually there are two images associated with an operator: one relating to the basis, the other relative to the inverse basis. As particular examples of the \( \hat{B}'s \) we may take three of the most useful bases, where
\[ \hat{B}(u,v) = \hat{t}(u,v), \quad \hat{B}^{-(u,v)} = \hat{t}(-u,-v) \] (2.7)
\[ \hat{A}(p,q) = \hat{\alpha}(p,q)/h^{3/2}, \quad \hat{A}^{-(p,q)} = \hat{\alpha}(p,q) \] (2.8)
\[ \hat{B}(p,q) = \hat{\beta}^{+(p,q))/h^{3/2}, \quad \hat{B}^{-(p,q)} = \hat{\beta}^{-(p,q)} \] (2.9)
The existence of an inverse basis is essential. The other properties of a particular basis are useful for special reasons, as symmetry, Planck-constant dependence, rapid convergence of integrals, etc. If possible, the symmetry properties of the problem should be shifted as much as possible into the basis. For example, a general physical situation is symmetric under displacement in the \( \hat{p} \) and \( \hat{q} \) operators. The displacement in \( \hat{q} \) follows from not having a preferred point in space, and the displacement in \( \hat{p} \) is the consequence of Galilean invariance, and gauge invariance. The \( \hat{t} \) and \( \hat{\alpha} \) bases embody this symmetry. The Planck constant dependence of the images is also important. The operator nature of the operators is carried in the operator nature of the basis. Since the dependence on Planck's constant is a consequence of dealing with operators, one expects to remove much of the Planck constant dependence working with the images. The choice of basis will determine the actual Planck constant dependence of the images. Weyl,
for example believed (incorrectly) that the \( \hat{T} \) basis removes the Planck constant dependence altogether, and he based his quantization rule (construction of operators associated with classical dynamical quantities) on this belief. He Fourier analyzed a classical dynamical quantity, and used the resulting expansion coefficient (which of course is independent of Planck's constant) as the expansion coefficient of the quantum mechanical operator. Wigner used the \( \hat{A} \) basis to associate a function, Wigner's function, with the density operator. He implied that the expansion coefficients, Wigner's function, is a power series in Planck's constant and hence is analytical in it. This, however, is not true in general. A list of conditions which specifies uniquely Wigner's function (hence the \( \hat{A} \) basis) is given by O'Connell and Wigner (1981).

Given an association in the \( p,q \) variables, the following property (if present) is very useful. Integrating the image of the density operator with respect to \( p \) or \( q \) should give the actual probability distribution of the remaining variable, i.e. the diagonal element of the density matrix in the corresponding \( q \), or \( p \) representation. In the language of mathematical statistics they should form a marginal distribution. Moreover, this property should persist if we subject both \( p,q \) and the parameters \( p,q \) to an arbitrary unimodular transformation, since these are the simplest transformations which mix the \( p \) and \( q \) operators and still leave the commutation relations invariant. The \( \hat{A} \) basis actually has this property, while the \( \hat{A}_K \) basis does not.

Summary: We can associate functions with an operator in many different ways. In the present context it is useful to proceed in the following manner. We write any dynamical operator \( \hat{A}(\hat{p},\hat{q}) \) as a linear combination of a set of operators \( \hat{B}(\hat{p},\hat{q};a,b) \) which forms a basis set of operators
enumerated by the c-number labels a, b. In terms of the expansion coefficients $A_B(a, b)$ the operator $\hat{A}(\hat{p}, \hat{q})$ can be written as $\int dadb A_B(a, b) \hat{B}(\hat{p}, \hat{q}; a, b)$; $A_B(a, b)$ are the functions we associate with the dynamical operator $\hat{A}$. Wigner's function, and other functions used in semiclassical methods arise in this way through a particular choice of $\hat{B}(\hat{p}, \hat{q}; a, b)$.

2.3 The Three Common Bases

Now we return to the more detailed discussion of the properties associated with the three bases $\tilde{A}$, $\hat{A}$, $A_K^*$, given as examples in Eqs. (2.7-2.9). In these bases the same operator $\hat{A}(\hat{p}, \hat{q})$ can be written as

$$\hat{A}(\hat{p}, \hat{q}) = \int d^3ud^3v \tilde{A}(u, v) \hat{B}(u, v) = \int d^3p d^3q A_W(p, q) \hat{A}(p, q)/\hbar^3$$

$$= \int d^3p d^3q A_K^*(p, q) \hat{A}_K(p, q)/\hbar^3. \quad (2.10)$$

where the expansion coefficients $\tilde{A}(u, v), A_W(p, q), A_K^*(p, q)$ are the functions associated with the same operator $\hat{A}$. These functions are displayed in different spaces, the corresponding parameter spaces.

That these spaces are different is also reflected in the different physical meaning of the parameters. The $u, v$ space is the least transparent physically. It is the reciprocal or dual space associated with the $p, q$ space used to display $A_W(p, q)$. The $p, q$ space associated with the $\tilde{A}$ basis and the $p, q$ space associated with the $A_K^*$ basis are not the same since their geometrical structure is different. (They are invariant under different groups of transformations.) However, they both reduce to the classical phase space as $\hbar \to 0$. Hence, in this limit the parameters $q$ and $p$ become the classical coordinates and conjugate momenta. Similarly, in this limit, the quantities $A_W(p, q), A_K(p, q)$ become the same, equal to the classical dynamical quantity represented in quantum mechanics by the operator $\hat{A}$. (All $p, q$ parameter spaces are...
so constructed that they should reduce to the classical phase space when \( n = 0 \).)

**The \( \hat{T} \) basis, or Weyl basis**

The usefulness of the \( \hat{T} \) basis resides in the simple relations this basis exhibits, and which are also at the root of the more complicated relations satisfied by the \( \hat{A} \) and \( \hat{A}^\dagger \) bases. We shall now discuss these relations. (They are collected and listed for easy reference in Appendix II.1.)

The \( \hat{T} \) basis or Weyl basis is defined as

\[
\hat{T}(u,v) = e^{i(u \cdot \mathbf{p} + v \cdot \mathbf{q})}. \tag{2.11}
\]

We now establish the inverse basis, and the composition law for functions associated with operator products. From the definition it immediately follows that

\[
\text{Tr}(\hat{T}(u,v)) = \left(\frac{2\pi}{\hbar}\right)^3 \delta(u)\delta(v). \tag{2.12}
\]

The \( \hat{T} \) operator set also satisfies the duplication formula

\[
\hat{T}(u,v)\hat{T}(u',v') = \exp\left[(i\hbar/2)(u \cdot \mathbf{p}' - v \cdot \mathbf{q}')\right] \hat{T}(u+u',v+v'). \tag{2.13}
\]

Taking the trace of this expression we find

\[
\text{Tr}(\hat{T}(u,v)\hat{T}(-u',-v')) = (2\pi/\hbar)^3 \delta(u-u')\delta(v-v'). \tag{2.14}
\]

Comparing this with Eq. (2.2) we immediately see that the inverse of the basis \( \hat{T}(u,v) \) is given by \( \hat{T}(-u,-v) (\hbar/2\pi) \) (see Appendix II.1).

The duplication formula expresses the product of two \( \hat{T} \) operators as a single \( \hat{T} \) operator. This can be used to obtain the composition law for the functions \( \hat{A}\hat{B}(u,v) \) associated with the operator \( \hat{\lambda}\hat{\beta} \) in terms of the functions \( \hat{\lambda}(u,v), \hat{\beta}(u,v) \) associated with the individual operators \( \hat{A}, \hat{B} \) appearing in the product \( \hat{\lambda}\hat{\beta} \). (Express \( \hat{\lambda}, \hat{\beta} \) and \( \hat{\lambda}\hat{\beta} \) in terms of \( \hat{T} \), and equate the expansion coefficients using the duplication formula.) We find
\[(\hat{A}\hat{B})(u,v) = \int d^3u'd^3v'\hat{A}(u',v')\hat{B}(u-u',v-v') \times \]
\[\times \exp[(i\hbar/2)(u\cdot v' - v\cdot u')] . \quad (2.15)\]

We notice that if \(\hbar=0\) we obtain the standard convolution expression as expected for the Fourier coefficients of factors in a product of the functions expanded. Thus all the complications stem from the phase factor in the duplication formula.

The \(\hat{\alpha}\) basis or Wigner's basis

The \(\hat{\alpha}(p,q)\) basis is defined as
\[\hat{\alpha}(p,q) = (\pi/2\pi)^3 \int d^3d^3\hat{\alpha} \exp[i(u\cdot p+u\cdot q)]\hat{\alpha}(-u,-v) . \quad (2.16)\]

We now establish the inverse basis, then specify the composition law. Finally we express the \(\hat{\alpha}\) basis in the \(x\) representation to exhibit the relation with the usual definition of Wigner's function. An extensive list of useful formulæ will be in Appendix II.2.

Using the definition of \(\hat{\alpha}\) in terms of \(\hat{\alpha}\) and the expression for the trace of \(\hat{\alpha}\), we immediately find
\[\text{Tr}\hat{\alpha}(p,q) = 1 \quad (2.17)\]
\[\text{Tr}(\hat{\alpha}(p,q)\hat{\alpha}(p',q')) = (2\pi\hbar)^3\delta(p-p')\delta(q-q') . \quad (2.18)\]

Consequently the inverse basis to \(\hat{\alpha}(p',q')\) is \(\hat{\alpha}(p',q')/(2\pi\hbar)^3\).

We can express the product of \(\hat{\alpha}\) operators using the composition law already obtained for the the \(\hat{\alpha}\) operator and we find
\[\hat{\alpha}(p,q)\hat{\alpha}(p',q') = \left(\frac{4}{2\pi\hbar}\right)^3\int d^3p''d^3q''\exp\left\{-\frac{2i}{\hbar}p''|p,q\rangle\langle p',q'|p''\right\}\hat{\alpha}(p'',q''), \quad (2.19)\]

This expression corresponds to the simple duplication formula for the \(\hat{\alpha}\) operators. The particular simplicity of the \(\hat{\alpha}\) basis arose from the fact that the product of \(\hat{\alpha}\) operators is proportional to a single \(\hat{\alpha}\) operator, while the product of two \(\hat{\alpha}\) operators is a linear combination of an infinite number of \(\hat{\alpha}\) operators.
The above formula can now be used to establish the composition law for functions associated with products of two operators, in terms of the functions associated with the operators in the product using the \( \hat{A} \) basis. This way one finds that if \( \hat{O} = \hat{A}\hat{B} \), then

\[
C_{\hat{O}}(p,q) = \frac{1}{(4\pi)^6} \int d^3p' d^3q' d^3p'' d^3q'' \exp \left\{ -\frac{2i}{\hbar} \left| \frac{p'q''}{pqr} \right| \right\} \times A_{\hat{A}}(p',q') B_{\hat{B}}(p'',q'').
\]

(2.20)

It is possible to transform this expression into the more familiar one involving derivatives of infinite order

\[
C_{\hat{O}}(p,q) = \exp \left\{ \frac{2i\hbar}{\pi} \left( q_A \cdot p - q_B \cdot p - q_A \cdot q_B \right) \right\} A_{\hat{A}}(p_A,q_A) B_{\hat{B}}(p_B,q_B)
\]
evaluated at

\[
p_A = p_B = p, \quad q_A = q_B = q.
\]

(2.21)

However, for pedagogical purposes it is useful to rederive this result directly, showing this way that the derivatives arise as a simple consequence of the phase factor in the duplication formula of the \( \hat{A} \) operators.

From Eq. (2.15) giving \( \hat{A}\hat{B} \) in terms of \( \hat{A} \) and \( \hat{B} \) we find

\[
C_{\hat{O}}(p,q) = \int d^3u d^3v e^{i(u^*p + v^*q)} \tilde{\hat{A}}(u,v) = \int d^3u d^3v d^3u' d^3v' e^{i(u^*p + v^*q)} \times
\]

\[
\times \tilde{\hat{A}}(u',v') \tilde{\hat{B}}(u-u',v-v') e^{i(\hbar/2) (u^*v' - v^*u')}.
\]

(2.22)

The phase factor at the end containing \( \hbar \) is just the phase factor in the duplication formula. If it were missing, the variable transformation \( u'' = u - u', \quad v'' = v - v' \) would immediately lead to the result \( C_{\hat{O}}(p,q) = A_{\hat{A}}(p,q) B_{\hat{B}}(p,q) \), as expected. Let us use the same transformation with the phase factor being present. We find

\[
C_{\hat{O}}(p,q) = \int d^3u' d^3v' d^3u'' d^3v'' \tilde{\hat{A}}(u',v') e^{i(u'^*p + v'^*q)} \tilde{\hat{B}}(u'',v'') e^{i(u''^*p + v''^*q)} \times e^{i(\hbar/2) (u''^*v' - v''^*u')}.
\]

(2.23)
Introduce now the auxiliary quantity \( C(p_A^q, p_B^q) = \int d^3u^d^3v^d^3u'd^3v' \)
\[ \tilde{A}(u', v') e^{i(u' \cdot p_A^q + v' \cdot q_A)} \delta(u'' - v'' - u') e^{i(u'' \cdot p_B^q + v'' \cdot q_B)} i(\hbar/2)(u'' \cdot v'' \cdot u') \]. We notice that
\[
C_{AB}(p_A^q, p_B^q) = C(p, q) \quad (2.24)
\]
Expand now the last exponential in \( C_{AB} \) into powers of \( \hbar \).
\[
\exp\{(i\hbar/2)(u'' \cdot v'' \cdot u')\} = 1 + (i\hbar/2)(u'' \cdot v'' \cdot u') + \ldots \quad (2.25)
\]
\( C_{AB} \) will be a sum of integrals. The first integral containing the term 1 is trivial; the next contains the term \( i(\hbar/2)(u'' \cdot v'' \cdot u') \).

This factor can also be generated by differentiating the exponentials
\[
e^{i(u'' \cdot p_A^q + v'' \cdot q_A)} e^{i(u'' \cdot p_B^q + v'' \cdot q_B)} \]
i.e. applying the operator \(-i(\hbar/2)(\partial\partial\partial\partial q_A - \partial\partial\partial\partial q_A) - \partial\partial\partial\partial p_A \partial\partial\partial\partial q_B)\) to the integral. Similarly all the terms can be generated by applying powers of this operator. This way we find that
\[
C_{AB} = \exp\{-i(\hbar/2)\left(\frac{\partial}{\partial p_B} - \frac{\partial}{\partial q_A} - \frac{\partial}{\partial p_A} \right)\} \hat{A}_W(p_A q_A) \hat{W}(p_B q_B) \quad (2.26)
\]
Before leaving the W transform we want to show that the formula \( A^W = \text{Tr}(\hat{A} \hat{A}) \) reduces to the usual form for the Wigner function. To do this we need \( \hat{A} \) in the \( x \) representation. This is easily found from the \( x \) representation of the \( \hat{A} \) operator [Eq. (AIII.11)]. We have thus
\[
<x|\hat{A}(p, q)|x'> = \delta(q - \frac{x+x'}{2}) e^{i(x-x') \cdot p/\hbar} \quad (2.27)
\]
and \( A^W \) can be written
\[
A^W = \int d^3 x d^3 x' \delta(q - \frac{x+x'}{2}) e^{i(x-x') \cdot p/\hbar} <x'|\hat{A}|x> = \int d^3 s e^{is \cdot p/\hbar} <q - \frac{1}{2} s|\hat{A}|q + \frac{1}{2} s> \quad (2.28)
\]
In the special case when \( \hat{A} \) is the density matrix \( \rho \) we have the usual definition of Wigner's function
\[
f_W(p, q) = \int d^3 s e^{is \cdot p/\hbar} \rho(q - \frac{1}{2} s, q + \frac{1}{2} s) \quad (2.29)
\]
We note that \( A^W \) will be real if \( \hat{A} \) is Hermitian; hence \( f_W(p, q) \) is real.
At this level an expression of this kind is the inevitable consequence of using the $\hat{T}$ basis in our operator space. The question, however, arises whether the particular structure of this formula could also be understood by other, more intuitive means? After all, Wigner has not obtained it in this manner. A simple heuristic explanation will be given in Appendix II.3. [The literature discussing the basic properties of Wigner's function is very large. (This arises, partially, because the relation of these properties to the duplication formula (2.13) is often not realised.) See, e.g. Groenewold 1946; Irving and Zwanzig 1951; Baker 1958; Mori, Oppenheim and Ross 1962; Cohen 1964, 1966; Mehta 1964; Leaf 1968; Agarwal and Wolf 1970a,b,c; deGroot 1974; Amiet and Huguenin 1981.]

The $\hat{A}^+,-, basis or Kirkwood basis

We now proceed to the $\hat{A}^+$ basis, the last of the three bases which we will explore in detail. This basis is discussed for several reasons; first because we will use it in Section 3 in actual calculations; next, to stress the non-uniqueness of the choice of bases; and finally because it is fairly widely used in the literature (Kirkwood 1933; Mehta 1964) although it has not been recognized that the algorithm presented is nothing but a different choice of basis.

The $\hat{A}^+_K(p,q)$ is defined by

$$\hat{A}^+_K(p,q) = (2\pi)^3 \delta(p-p) \delta(q-q) = \left(\frac{\hbar}{2\pi}\right)^3 \int d^3u d^3v \hat{A}(u,v) \exp\{-i(u \cdot p + v \cdot q)\} \times \exp\left(i\frac{\mu u \cdot v}{2}\right).$$

(2.30)

(An extensive list of formulae is again given in Appendix II.2) The use of this basis is slightly complicated by the fact that the inverse basis, $\hat{A}^-_K$, is not the same as $\hat{A}^+_K$; it is given by
That this is actually the inverse basis is easily verified by using the properties of the $\hat{T}$ operators. The $\hat{\Delta}_K^*$ and $\hat{\Delta}_K$ are Hermitian conjugates of each other. Since they are different a second set of expansion coefficients can be defined by

$$\hat{\Lambda} = \int \frac{d^3p}{(2\pi)^3} A_K^-(p,q) \hat{\Delta}_K(p,q).$$

(2.32)

It is a matter of taste which of $\hat{\Delta}_K^*$, $\hat{\Delta}_K$ one chooses as the direct basis; the other one being then the inverse basis. Unlike the $A_w(p,q)$ functions which are always real for $\hat{\Lambda}$ Hermitian, the $A_K^+$ and $A_K^-$ are in general complex even for Hermitian operators, save in the classical limit, when they also reduce to the classical dynamical quantity represented by $\hat{\Lambda}$. (However, the sum $\hat{\Delta}_K^* + \hat{\Delta}_K^-$ is real for $\hat{\Lambda}$ Hermitian. Indeed, this quantity used as an associated function has been implied in the work of Rivier (1951). We shall return briefly to its discussion after settling the Kirkwood basis.)

As with the $\hat{\Lambda}$ basis the composition rule can be easily found using the duplication formula for the $\hat{T}$ operators. If we take $C=AB$ then

$$C_{K}^+(p,q) = \int \frac{d^3p \cdot d^3q}{h^3} A_{K}^+(p,q') B_{K}^+(p',q) \exp\left\{ -\frac{i}{\hbar}(p-p')(q-q') \right\}$$

$$\exp\left\{ i \cdot \frac{q}{p} \cdot v \cdot \frac{q}{p} \cdot v \right\} A_{K}^+(p_a,q_a) B_{K}^+(p_b,q_b)$$

(2.33)

where the derivatives are evaluated at $p_a = p_b = p$ and $q_a = q_b = q$. The corresponding expression for $C_{K}^-$, $A_{K}^-$ and $B_{K}^-$ has the $i$'s in the exponentials replaced by $(-i)$'s and the arguments of $A$ and $B$ interchanged.

The Kirkwood basis is given in the $x$ representation as

$$\langle x' | \hat{\Delta}_K^* | x'' \rangle = \delta(x''-q) \exp\left\{ i(x''-q) \cdot p/\hbar \right\}. \tag{2.34}$$

Hence evaluating $\text{Tr}(\hat{\Lambda} \hat{\Delta}_K^+)$ we find

$$A_{K}^-(p,q) = e^{-iq \cdot p/\hbar} \int q | \hat{\Delta} | x' \rangle e^{ix' \cdot p/\hbar} d^3x' \tag{2.35}$$
where $\langle q|\hat{A}|x'\rangle$ is the matrix element of $\hat{A}$ in the $x$ representation. We notice now that $e^{ix\cdot p/\hbar}$ and $e^{-iq\cdot p/\hbar}$ can be written as $(2\pi)^{3/2}\langle x'|k\rangle$ and $(2\pi)^{3/2}\langle k|q\rangle$, where $\langle x'|k\rangle$ is the transformation coefficient going from the $x$ to the momentum representation and $k=p/\hbar$. Thus we can immediately write

$$A_k^+(p,q) = (2\pi)^{3/2}\langle k|q\rangle \langle q|\hat{A}|k\rangle,$$  \hfill (2.36)

showing that $A_k^+(p,q)$ is proportional to the matrix element of $\hat{A}$ in the mixed representation $\langle x'|\hat{A}|k\rangle$ replacing $k'$ by $q$, $\xi k'$ by $p$. This form is attractive, since the matrix elements in the mixed representation can be usually simply evaluated, especially if the operator is a polynomial in $p$ and $q$.

We now establish the relation between the expansion coefficients of $\hat{A}$ relative to the $A_k^+$ and $A_k^-$ bases, i.e. the relation between the functions $A_w(p,q)$ and $A_k(p,q)$. To change the components of a vector under coordinate transformations we need to know the direction cosines, i.e. the scalar products of a basis vector in one frame, with the (inverse) basis vector of the other frame. Here this corresponds to the quantities $\text{Tr}(\hat{A}(p',q')A_k^-(p,q))$. Indeed, knowing these quantities we proceed as follows:

$$A_w(p',q') = \text{Tr}(\hat{A}(p',q')\hat{A})$$  \hfill (2.37)

$$A_k^-(p,q) = \text{Tr}(\hat{A}_k(p,q)\hat{A})$$  \hfill (2.38)

$$\hat{A} = \int \frac{d^3p'd^3q'}{(2\pi)^3} A_w(p',q')\hat{A}(p',q')$$  \hfill (2.39)

$$\hat{A} = \int \frac{d^3p'd^3q'}{(2\pi)^3} A_k^-(p',q')\hat{A}_k^+(p',q').$$  \hfill (2.40)

Now express $A_w$ using under the trace $\hat{A}$ as expressed in terms of $A_k^-$ and express $A_k^+$ using under the trace $\hat{A}$ as expressed in terms of $A_w$. We immediately find
The required quantity, \( \text{Tr}(\hat{\Delta}(p',q') \hat{\Delta}_{K}(p,q)) \), can immediately be evaluated, if we write \( \hat{\Delta}, \hat{\Delta}_{K} \) in terms of the \( \hat{T} \) operator; use the duplication formula in the product, and take the trace. We find

\[
\text{Tr}(\hat{\Delta}(p',q') \hat{\Delta}_{K}(p,q)) = 2^3 e^{2i(p'-p) \cdot (q'-q)/\hbar}.
\]

Consequently

\[
\text{Tr}(\hat{A}(p',q') \hat{\Delta}_{K}(p,q)) = 2^3 e^{2i(p'-p) \cdot (q'-q)/\hbar}.
\]

and similarly for \( \hat{A}^{\dagger}(p',q') \times \hat{\Delta}_{K}(p,q) \). Since \( \hat{A}^{\dagger}_{K}(p,q) \) can often be computed more easily by direct means than \( \hat{A}_{W}(p,q) \), this relation can be used to find \( \hat{A}_{W}(p,q) \). This expression also shows that \( \hat{A}_{W} \) and \( \hat{A}^{\dagger}_{K} \) become the same in the \( \hbar \to 0 \) limit. Notice that we have from Eq. (2.43-2.44)

\[
\hat{A}^{\dagger}_{K}(p,q) = 2^3 d^{3}p' d^{3}q' \hat{\Delta}(p',q') \exp\left\{ \frac{i}{\hbar} [2(p'-p) \cdot (q'-q)/\hbar] \right\}.
\]

In Table II.2 we give some simple examples of image functions for both the \( W \) and Kirkwood associations. As expected the different image functions agree only to lowest order in \( \hbar \). This is also true for the commutators. For lowest order in \( \hbar \) the commutator is just a Poisson bracket; the correction terms of higher order in \( \hbar \) depend on the choice of basis and hence are not unique. This is due to the lack of uniqueness in how the phase space is extended to the quantum mechanical problem. Of course the higher order terms become unique once a basis is chosen. It then makes no sense in the abstract to ask what are the quantum corrections to Poisson brackets without specifying the basis.
For example in the Kirkwood representation we have that
\[
C_K^+ = \exp\left\{ i\left( \frac{p_2}{\hbar} \cdot \mathbf{v} - \frac{q_1}{\hbar} \cdot \mathbf{v} \right) \right\} \exp\left\{ i\left( \frac{p_1}{\hbar} \cdot \mathbf{v} - \frac{q_2}{\hbar} \cdot \mathbf{v} \right) \right\} A_K^+(p_1, q_1) B_K^+(p_2, q_2)
\] (2.47)
where \( \hat{C} = [\hat{A}, \hat{B}] \) and the derivatives are evaluated at \( p_1 = p_2 = p \) and \( q_1 = q_2 = q \). In the Wigner case we have
\[
C_W = 2i \sin(\hbar^2/2) \left( \frac{v}{p_2} \cdot \frac{q_1}{p_1} - \frac{v}{p_1} \cdot \frac{q_2}{p_2} \right) A_W(p_1, q_1) B_W(p_2, q_2)
\] (2.48)

Summary: In this section we discuss the properties of three bases, \( \hat{A}(p, q) \), \( \hat{A}_K(p, q) \), \( \hat{T}(u, v) \) (the dependence on \( \hat{p}, \hat{q} \) is not indicated).

If we expand the density operator in the basis \( \hat{A}(p, q) \) we obtain as the expansion coefficients \( f_W(p, q) \), Wigner's function; \( \hat{A}_K(p, q) \) leads to Kirkwood's function; \( \hat{T}(u, v) \) (suggested by Weyl) leads to the Fourier transform of Wigner's function. The formal properties of each function are determined by the properties of each basis set; their relations to each other are determined by the relations of the corresponding basis sets to each other.
Table II.2

<table>
<thead>
<tr>
<th>$\hat{p}$</th>
<th>$\Lambda^-_K$</th>
<th>$\Lambda^+_K$</th>
<th>$\Lambda_W$</th>
</tr>
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<tr>
<td>$p$</td>
<td>$p$</td>
<td>$p$</td>
<td>$p$</td>
</tr>
<tr>
<td>$q$</td>
<td>$q$</td>
<td>$q$</td>
<td>$q$</td>
</tr>
<tr>
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<td>$f(p)$</td>
<td>$f(p)$</td>
<td>$f(p)$</td>
</tr>
<tr>
<td>$f(q)$</td>
<td>$f(q)$</td>
<td>$f(q)$</td>
<td>$f(q)$</td>
</tr>
<tr>
<td>$p \cdot q$</td>
<td>$p \cdot q - 3\imath\hbar$</td>
<td>$p \cdot q$</td>
<td>$p \cdot q - 3\imath\hbar/2$</td>
</tr>
<tr>
<td>$q \cdot p$</td>
<td>$p \cdot q$</td>
<td>$p \cdot q + 3\imath\hbar$</td>
<td>$p \cdot q + 3\imath\hbar/2$</td>
</tr>
<tr>
<td>$(q \cdot p - p \cdot q)$</td>
<td>$3\imath\hbar$</td>
<td>$3\imath\hbar$</td>
<td>$3\imath\hbar$</td>
</tr>
<tr>
<td>$\hat{p} f(q) \hat{p}$</td>
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<td>$p^2 f(q) + \imath \hbar p \cdot Vf(q)$</td>
<td>$p^2 f(q) + (\hbar^2/4) V^2 f(q)$</td>
</tr>
<tr>
<td>$f(q) \hat{p}^2$</td>
<td>$p^2 f(q)$</td>
<td>$p^2 f(q) + 2\imath \hbar p \cdot Vf(q)$</td>
<td>$p^2 f(q) + \imath \hbar p \cdot Vf(q)$</td>
</tr>
<tr>
<td>$\hat{p}^2 f(q)$</td>
<td>$p^2 f(q) - 2\imath \hbar p \cdot Vf(q)$</td>
<td>$p^2 f(q)$</td>
<td>$p^2 f(q) - \imath \hbar p \cdot Vf$</td>
</tr>
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<td>$-(\hbar^2/4) V^2 f(q)$</td>
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<td></td>
</tr>
<tr>
<td>$1/4 (\hat{p}^2 f(q) + f(q) \hat{p}^2)$</td>
<td>$p^2 f(q) - \imath \hbar p \cdot Vf(q)$</td>
<td>$p^2 f(q) + \imath \hbar p \cdot Vf$</td>
<td>$p^2 f(q)$</td>
</tr>
<tr>
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<td>$-(\hbar^2/4) V^2 f(q)$</td>
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<tr>
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<tr>
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<td>$+(\hbar^2/4) V^2 f(q)$</td>
<td></td>
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</tbody>
</table>
2.4 Bases Specified Through Ordering

We have discussed three operator bases introducing the operator sets $\hat{T}(u,v)$, $\hat{A}(p,q)$, and $\hat{A}_K(p,q)$. These were essentially the bases suggested by the work of Weyl, Wigner, and Kirkwood. There is, however, an alternative way to introduce different basis sets, noticing that the ordering of the $\hat{p}$ and $\hat{q}$ operators in the bases lead to changes in those bases. Accordingly, we shall now reinterpret these bases in terms of ordering and suggest the possibility of constructing alternative bases using other types of ordering. (See e.g. Shewell 1959; Sudarshan 1963; Mehta 1964; Cohen 1966.)

For example we may write the Kirkwood basis $\hat{A}_K(p,q)$ as

$$\hat{A}_K(p,q) = h^3\delta(\hat{p}-p)\delta(\hat{q}-q).$$

From this we see immediately that the Kirkwood basis corresponds to that ordering of the $\hat{p}$ and $\hat{q}$ operators in the basis, in which the $\hat{q}$ operators act first, and the $\hat{p}$ operators after that. This is the usual standard ordering. Thus the Kirkwood basis is the basis associated with the standard ordering of $\hat{p}$ and $\hat{q}$ and the inverse Kirkwood basis corresponds to the anti-standard ordering of $\hat{p}$ and $\hat{q}$. Other bases can be obtained from the Kirkwood one by using a different ordering of the $\hat{p}$ and $\hat{q}$ operators in the delta function product, or in the exponents.

The $\hat{A}$ bases imply a different ordering, which may be called the Weyl ordering or equivalently one may say $\hat{A}$ is the Weyl ordered delta function. It is difficult to specify this reordering for the delta operators; however, it is simple to do so for the Fourier components and leads simply to a multiplication by a phase (see Table II.1). The effects of the Weyl-ordering can be easily shown on polynomials. If we have $\hat{p}^m \hat{q}^n$ the corresponding operator consists of taking the opera-
tor $\hat{p}$ $m$ times, the operator $\hat{q}$ $n$ times, putting them in all possible permutations with equal weights and dividing by the number of terms.

For example, if $m=n=2$ we have

$$\int \frac{d^3p}{h^3} \frac{d^3q}{h^3} \hat{A}(p,q)p^{2q^2} = \frac{1}{6} \{\hat{p}\hat{p}\hat{q}\hat{q} + \hat{p}\hat{q}\hat{q}\hat{p} + \hat{q}\hat{p}\hat{p}\hat{q} + \hat{q}\hat{q}\hat{p}\hat{p} + \hat{q}\hat{q}\hat{q}\hat{p} + \hat{q}\hat{p}\hat{q}\hat{p}\} \} \quad (2.49)$$

which with the help of the commutation relations may be rewritten

$$\int \frac{d^3p}{h^3} \frac{d^3q}{h^3} \hat{A}(p,q)p^{2q^2} = \frac{1}{4} \{\hat{p}^2\hat{q}^2 + \hat{q}^2\hat{p}^2 + 2\hat{p}\hat{q}\} \quad (2.50)$$

in agreement with line 11 of Table II.2 (take $f(q)=q^2$).

An alternative ordering which is used is the normal ordering. In this case one defines creation and annihilation operators $\hat{a}$ and $\hat{a}^+$ by

$$\hat{a}^+ = \frac{1}{\sqrt{2}} \left[ (m\omega)^{1/2} \hat{q} - \frac{1}{(m\omega)^{1/2}} \hat{p} \right] \quad (2.51)$$

$$\hat{a} = \frac{1}{\sqrt{2}} \left[ (m\omega)^{1/2} \hat{q} + \frac{1}{(m\omega)^{1/2}} \hat{p} \right] \quad (2.52)$$

where $m$ and $\omega$ are fixed but arbitrary parameters. Normal ordering consists of putting the creation operators $\hat{a}^+$ before the annihilation operators $\hat{a}$. We show in Appendix II.4 that this can be done through the introduction of a new delta

$$\delta_{N}^{\pm}(p,q) = \frac{\hbar^3}{(2\pi)^3} \int d^3u d^3v \exp\{-i[u*(p-\hat{p})+v*(q-\hat{q})]\} \exp\{\frac{1}{4} \left( \frac{v^2}{m\omega} + m\omega^2 \right) \} \quad (2.53)$$

We then have

$$\hat{A}^+_{N}(p,q) = \text{Tr} \hat{A}^+_N(p,q) \quad (2.54)$$

and

$$\hat{A} = \frac{1}{\hbar^3} \int d^3p d^3q \hat{A}^+_N(pq)\hat{A}^+_N(pq) \quad (2.55)$$

More details, as well as additional properties of this association are given in Appendix II.4. Here we just wish to stress two points. First, that this different ordering corresponds simply to another basis, and secondly, since $m\omega$ is arbitrary we actually generate an infinite number of different orderings or associations.

As we can introduce new bases, we can introduce new orderings since each new basis corresponds to a new ordering. However, not all...
Orderings are suitable for the generation of a basis, since we may not be able to construct the inverse basis. For example, the Rivier ordering is specified by using $1/2[\hat{A}_K(p,q)+\hat{A}_K(p,q)]$ as the putative $\hat{A}_R$ basis, or equivalently introducing $\hat{A}_R = \hat{T}(u,v)\cos(\kappa uv/2)$. It is immediately clear that there is no inverse due to the zeros in the cosine factor. Note that the Rivier ordering arises from the simplest method of generating a Hermitian delta from the Kirkwood delta. Another association or ordering which has the same problem is the Born-Jordan ordering [Amiet and Huguenin 1981]. There we have

$$\hat{T}_{BJ} = \frac{\sin(\kappa u - v/2)}{(\kappa u - v/2)}.$$  \hspace{2cm} (2.56)

Again no inverse exists because of the zeros in the factor multiplying the $\hat{T}(u,v)$. In general, this puts a restriction on the function used in the definition of $\hat{T}_F(u,v)$ in Table II.1, i.e.

$$\hat{T}_F(u,v) = \exp(i(u*p+v*q)F(u,v)).$$  \hspace{2cm} (2.57)

The $F(u,v)$ can have no zeros on the finite real $u,v$ axis. Zeros at infinity cause problems as in the case of normal ordering but these are not fatal. Each new choice of $F(u,v)$ which satisfies the above conditions will generate a new basis and a new ordering.

**Summary:** Operator bases can be selected for different reasons. A particular choice of ordering of the non-commuting operators $\hat{P}$ and $\hat{Q}$ may lead to a choice of basis. The Kirkwood basis $\hat{A}_K$ corresponds to the standard ordering, $\hat{A}_K$ to the antistandard ordering; the $\hat{A}(p,q)$ basis and the $\hat{T}(u,v)$ basis correspond to the Weyl ordering. The normal ordering corresponds to the basis $\hat{A}_N(p,q)$ which is equivalent to the coherent state representation. The ordering conceived by Rivier, and the ordering conceived by Born and Jordan do not lead to a correct basis, because the bases induced have no inverse.
2.5 Images associated with density matrices

Wigner's function

Having discussed the general properties of the W association we now return to the special case of the W transform of the density matrix

\[ f_w(p,q) = \text{Tr}(\hat{A}(p,q)\hat{\rho}) = \int d^3s \langle q^+ \frac{1}{2} s | \hat{\rho} | q^- \frac{1}{2} s \rangle e^{-ip \cdot s/\hbar}. \]  

(2.58)

To avoid confusion we now define our normalization conventions.

For discrete states we have \( \text{Tr} \hat{\rho} = 1 \) corresponding to the conventional definition

\[ \int d^3x | \langle x | \psi \rangle |^2 = 1. \]  

(2.59)

In the W transform this gives

\[ \int d^3p d^3q f(p,q) = (2\pi \hbar)^3, \]  

(2.60)

corresponding to one state occupying a volume of \( \hbar^3 \) (not \( \pi^3 \)) in phase space. The \( f(p,q) \) is itself dimensionless. For pure (normalized) states this implies an idempotency condition on the density matrix, \( \hat{\rho}^2 = \hat{\rho} \). Using the composition rule for Wigner's function (Eq. AII2.15) this implies the following condition for \( f(p,q) \):

\[ \frac{1}{(2\pi \hbar)^3} \int d^3p d^3q d^3p' d^3q' d^3p'' d^3q'' \exp \left\{ \frac{2\pi}{\hbar} \begin{pmatrix} p' & q' & 1 \\ p & q & 1 \end{pmatrix} \right\} f(p',q')f(p'',q'') = f(p,q). \]

(2.61)

For states in the continuum \( \text{Tr}(\hat{\rho}) \) diverges but it is possible to use the orthogonality conditions to define the normalization if the wave function belongs to an orthogonal set. Label the orthogonal set by a continuous parameter for example the energy \( E \). The orthogonality condition is then

\[ \hat{\rho}(E)\hat{\delta}(E') = \hat{\delta}(E)\hat{\delta}(E-E') \]  

(2.62)

The normalization thus depends on choice of the parameter specifying the state. For Wigner's function this results in the relation...
We now proceed to discuss the general density matrix. If the density matrix is time-dependent, it satisfies the equation
\[ \frac{1}{\hbar} \frac{\partial \hat{\rho}}{\partial t} = [\hat{H}, \hat{\rho}] ; \] (2.64)
or, for \( f(p,q) \), the equation
\[ \frac{\partial f(p,q)}{\partial t} = \frac{2}{\hbar} \sin \frac{\hbar}{2} (\nabla \cdot \nabla - \nabla \cdot \nabla) \hat{H}(p_1,q_1)c f(p,q) \bigg|_{p_1=p} \bigg|_{q_1=q} . \] (2.65)

Here \( \hat{H}(p,q) \) is the \( \hat{W} \) transform of \( \hat{H} \). We have used the common differential expression for the composition rule, Eq. AII2.16, rather than the mathematically more correct integral expression of Eq. AII2.15. In the limit \( \hbar \to 0 \) the right-hand side reduces to a Poisson bracket. For a stationary state the above equation implies
\[ \sin \frac{\hbar}{2} (\nabla \cdot \nabla - \nabla \cdot \nabla) \hat{H}(p_1,q_1)c f(p,q) \bigg|_{p_1=p} \bigg|_{q_1=q} = 0 . \] (2.66)

A basic unresolved problem is the condition to be imposed on Wigner's function in order that it should represent a physically realizable state. In classical physics this condition asserts that \( f(p,q) \) be nowhere negative. In quantum mechanics the equivalent condition is that \( \hat{\rho} \) should have no negative eigenvalues. It is unclear what are sufficient conditions on \( f_W(p,q) \) such that the corresponding \( \hat{\rho} \) has this property. There are, however, necessary conditions. For example if \( f_W(p,q) \) is a delta function the argument must be linear and in \( p \) and \( q \) i.e. of the form \( ap+bq+c \) (Balazs 1980). One can also show that it is necessary (but not sufficient) that
\[ \int d^3p'd^3q' f_W(p',q') \exp[-(p'-p_0)^2/2\alpha^2-(q'-q_0)^2/2\beta^2]>0 \] (2.67)
with \( 2\alpha > \hbar \) if \( f_W \) corresponds to a physically realizable state.
(Iagolnitzer 1973). This follows from the observation that the integral is equal to \( \text{Tr}(\delta|p_0q_0><p_0q_0|) \) where \( <|p_0q_0> \) is the wave function of the ground state of a harmonic oscillator with Hamiltonian \((1/2)(p-p_0)^2 + (1/2)(q-q_0)^2 \) (see Appendix II.4). Other conditions of this form with other wave functions are of course possible. The extra condition on \( f_W \) to be physically realisable provides the escape route to avoid violating the uncertainty relations. Take for example \( f_W(p,q) \sim \delta(p-p_1)\delta(q-q_1) \). Then \( \Delta p \Delta q = 0 \), in seeming violation of the uncertainty relations. However, one can show that this \( f \) function does not correspond to a positive definite density operator.

For discrete states there are the further conditions (Baker 1958),

\[ |f_W(p,q)| < 2^3, \]  
(2.68)

and

\[ \int d^3p d^3q f_W^2(p,q) = (2\pi \hbar)^3. \]  
(2.69)

The generalization of Eqs. (2.68) and (2.69) for continuum states is unknown.

To develop a feeling for \( f(p,q) \) we now study some special cases. The dynamical systems will be one dimensional, and the associated \( (p,q) \) space two dimensional. Consider the plane wave state

\[ |x|k> = \frac{\delta_x}{(2\pi)^{1/2}} . \]  
(2.70)

The Wigner distribution for this state is

\[ f_W(p,q) = \hbar \delta(p-k) . \]  
(2.71)

We can also consider eigenfunctions of the more general operators \( aq + bp \) with eigenvalues \( \lambda; \) \((a,b, \) are scalars). The eigenfunctions are

\[ |\lambda> = \frac{1}{(2\pi \hbar)^{1/2}} \exp[-\frac{ia}{2\hbar}(x-\frac{\lambda}{a})^2] \]  
(2.72)

while Wigner's function is given by
First, note the form of the argument of the δ function. The δ function is singular on the line \(aq+bp=\lambda\). Linear, inhomogeneous transformations of \((p,q)\) leave a linear function linear, hence a line remains a line (and does not change into a curve). Consequently the functional form of this \(f(p,q)\) did not change under these transformations. While we demonstrated this on an \(f\) function which is a δ function, this is a transformation property of all Wigner functions, not shared by distribution functions obtained through other bases. Second, we note that the \(f\) function associated with an eigenstate of \(\hat{\mathbf{p}}\) (or \(\hat{\mathbf{q}}\)) is a δ function, and all \(f\)'s obtained from this one by linear transformations are then also δ functions. It turns out that these are the only Wigner functions which are δ functions and represent physically realizable states. All other Wigner functions have a finite width proportional to \(\hbar^{2/3}\). (See constant force case, Eq. 2.77.)

The next example we consider is two plane waves:

\[
\psi(x) = \frac{\exp(ikx + ik'x)}{(2\pi)^{1/2} (a^2 + b^2)^{1/2}}
\]  

(2.74)

where \(a\) and \(b\) are real. The Wigner function in this case is

\[
f(p,q) = \frac{\hbar}{a^2 + b^2} \left( a^2 \delta(p-\mathbf{k}) + b^2 \delta(p-\mathbf{k}') + 2ab \cos \frac{\hbar(k+k')}{\hbar} \right) \left( \delta(\mathbf{k}+\mathbf{k}' - p) \right).
\]

(2.75)

In this example there is a non-classical oscillatory term arising from the interference between the two terms. Thus, the superposition principle of states forces Wigner's function to take negative values. In the classical limit this interference term vanishes, albeit through infinitely rapid oscillations and not through the absolute value becoming small. Also notice that \(f(p,q)\) can be negative and hence it
is not a true probability. It is easy to see that the same conclusions hold if we replace the plane waves by WKB waves or gaussians.

The next example we consider is the one dimensional linear potential (Balazs, Zipfel 1973; Heller 1975). In this case the wave function is

$$\psi = \frac{1}{F} \left[ \frac{2mE}{h^2} \right]^{1/3} A_1 \left[ -(x+E/F) \left( \frac{2mE}{h^2} \right)^{1/3} \right]$$

(2.76)

where $F$ is the (constant) force. The corresponding Wigner function is

$$f(p,q) = \sigma A_1 \left( \sigma \left( \frac{p^2}{2m} - Fq - E \right) \right)$$

(2.77)

where $\sigma = (8m/F^2h^2)^{1/3}$. In this case we no longer have a zero width distribution but instead we have a width proportional to $h^{2/3}$. Hence in the classical limit we again obtain a zero width distribution. Wigner's function is peaked along the classically allowed energy surface

$$\frac{p^2}{2m} - Fq = E$$

(2.78)

On the side where

$$\frac{p^2}{2m} - Fq > E$$

(2.79)

the function decays exponentially; on the other side it oscillates with a slowly decreasing amplitude. This is a general feature of Wigner's function when the curves defined by $H(p,q) = E$ are not straight lines. As in the last example $f(p,q)$ can be negative. The integral

$$P_f(a,b,c) = \int dp dq \ \delta(qp+bq-c)f(p,q)/(2\pi h)$$

(2.80)

however, does define a probability and is positive for any value of $a$, $b$ and $c$. When $a=0$ this is just the ordinary coordinate space density. It is a remarkable property of Wigner's function that although in general it takes positive and negative values, its average along any line across the $p,q$ plane is positive. The fact that the oscillations in $f(p,q)$ always occur on the concave side of the curve $H(p,q) = E$ is related to the above positivity condition.
As the next example, we consider the one dimensional harmonic oscillator (see Groenewold 1946, Baker 1958). In this case
\[ \psi_n(x) = e^{-\frac{\omega x^2}{2\hbar}} H_n \left[ (\frac{\omega}{\hbar})^{1/2} x \right] \frac{1}{\left( \sqrt{\pi} n! \right)^{1/2}} \] (2.81)
and
\[ f(p,q) = (-1)^n 2e^{-2(p^2/2m+\omega q^2/2)/\hbar} \frac{1}{\pi n!} \left[ \frac{1}{2} + \frac{1}{2} \frac{\omega q^2}{\hbar} \right]. \] (2.82)
If we integrate over p and q we get just \( \hbar \) as we should. In this case, as in the case with the linear potential, \( f(p,q) \) depends on p and q only through \( H(p,q) \). This will no longer be true if we take a more complicated Hamiltonian. As in the previous case \( f(p,q) \) is peaked along \( H(p,q) = E \), decays exponentially for \( H(p,q) > E \) and oscillates for \( H(p,q) < E \). However, in the present case \( f(p,q) \) has a peak also at \( p=q=0 \). In fact it has its largest absolute value there
\[ f(0,0) = 2(-1)^n. \] (2.83)
However, the peak is sufficiently sharp that it gives relatively little contribution to any integrated quantity. The peaks in \( f(p,q) \) well inside the \( H(p,q) = E \) curve are a general feature when the \( H(p,q) = E \) curves are closed (see Berry 1980).

As an example of a very nonclassical system we consider a \( \delta \) function potential
\[ H = \frac{p^2}{2m} - \delta(q) \]. \] (2.84)
The wave function for the bound state is
\[ \psi(x) = e^{-\lambda|x|} \sqrt{\lambda} \] (2.85)
with \( \lambda = \frac{m\hbar^2}{\omega} \). Wigner's function for this state is given by
\[ f(p,q) = \frac{2e^{-2\lambda|q|}}{1 + e^{-2\lambda|q|}} \left( \cos \frac{2\lambda|q|}{\hbar} + \frac{i\hbar}{p} \sin \frac{2\lambda|q|}{\hbar} \right). \] (2.86)
Due to the discontinuity in the slope of \( \psi(x) \), \( f(p,q) \) does not decay exponentially for large values of \( p \) but only as \( p^{-2} \).
Kirkwood's function

Having discussed the Wigner representation of the density matrix in some detail we turn now to the Kirkwood representation for a pure state \( \psi \)

\[
 f_{K}^{-}(p,q) = \text{Tr}(\hat{A}^{\dagger} \hat{\rho}) = \hbar^{-3} \langle x' = q | \beta | k' = p/\hbar > \langle k' = p/\hbar | x' = q >
 = \hbar^{-3} \langle x' = q | \psi > \langle k' = p/\hbar | k' = p/\hbar | x' = q > .
\]

(2.87)

The normalization of \( f_{K}^{-}(p,q) \) is the same as that of \( f_{W}(p,q) \). The \( f_{K}^{-} \) function corresponding to a plane wave in one dimension is just

\[
 f_{K}^{-}(p,q) =\hbar \delta(p-hk) ,
\]

(2.88)

the same as for Wigner's function. However, the form of \( f_{K}^{-}(p,q) \) is not invariant under linear transformations of the \( p,q \) axes in the \( p,q \) plane and the \( f_{K}^{-} \) function associated with the state given by the wave function of Eq. (2.72) is:

\[
 f_{K}^{-}(p,q) = \frac{1}{(2\pi \hbar)^{1/2}} \exp \left[ -\frac{1}{2\hbar} (aq+bp-\lambda)^2 \right] .
\]

(2.89)

Note that the absolute value of this function is a constant. However, the phase is rapidly varying being stationary only on the line \( aq+bp-\lambda \).

Thus, this region will be the most important if we integrate over \( f \).

In the limit of \( \hbar \to 0 \) we will get a delta function but only through rapid oscillations. This is a fairly general feature of the \( f_{K} \) functions.

For the one dimensional linear potential we have

\[
 f_{K}^{-}(p,q) = \left( \frac{2m}{F^2\hbar^2} \right)^{1/3} \text{Ai} \left[ -(q+E/F) \left( \frac{2mE}{\hbar^2} \right)^{1/2} \right] \exp \left[ \frac{p^3}{6m\hbar} - \frac{pE}{m\hbar} - \frac{pq}{\hbar} \right] .
\]

(2.90)

We analyse this function more closely now to understand how the classical limit is reached. The absolute value of the function has its maximum on the line \( Fq+E=0 \); in addition, (as \( \hbar \) tends to zero) this function varies everywhere rapidly, save on the parabola \( p^2/2m-Fq=E \) where the phase of the function is stationary. This is the region...
occupied by the classical trajectory. The observed quantities are obtained as integrals of a smooth function multiplied with $f^\sim_K$.

Thus, we notice (a) that as $\hbar$ tends to zero, only regions near and on the classical trajectory will contribute to the integrals; (b) since in those integrals $f^\sim_K$ and not its absolute value enters, the region around the line $Fq+E=0$ gives small contributions only. In fact this line is a caustic, and as such has little to do with the classical limit. In appendix II.5 we show how these results arise.

For the one dimensional harmonic oscillator we have

$$f^\sim_K(p,q) = \frac{1^n}{\sqrt{\pi} 2^n n!} e^{-\left(p^2/2M+Z^2q^2/2\right)/\hbar \omega} \times$$

$$\times H_n(q/\sqrt{\hbar \omega})H_n(p/\sqrt{\hbar \omega})e^{-ipq/\hbar}$$

(2.91)

which is a somewhat less appealing expression than the corresponding Wigner's function.

As the last example let us consider the bound state of a delta function potential. Here we have

$$f^\sim_K(p,q) = \frac{2e^{-|q| |p| \hbar}}{(1+|p|^2/\hbar^2)}$$

(2.92)

which is simpler than the corresponding Wigner function.

The $f^\sim_K$ functions are in general more complicated than the corresponding Wigner functions. They are also complex and approach the classical limit through rapid oscillations.

The $f^\sim_3(p,q)$ functions; use of a new basis

Before leaving the images of density matrix we shall introduce a new basis, $\hat{\lambda}_3(p,q)$. The image of $\hat{p}$ generated by this basis, $f_3(p,q)$ will serve as a counter example to show that many of the properties exhibited by the Wigner and Kirkwood associations are not general ones but are the consequences of the particular bases used. Let us, then define a new basis $\hat{\lambda}_3(p,q)$ by
Again we consider motion in one dimension. This is a special case of the $\Delta_k(p, q)$ introduced previously now with $F = \exp[-i \frac{v^3}{3 \sigma_3 F_3^3}]$. (This is a cubic phase factor; hence the index 3.) For reasons of future convenience we put

$$\sigma_0 = \left(\frac{2m}{F^2}\right)^{1/3}. \quad (2.94)$$

In the limit $\sigma_0 \to 0$ the additional phase goes to zero.

The image function corresponding to the projection operator $\delta(q-q)$ is

$$f_3(p, q) \equiv \text{Tr} \left( \hat{\Delta}_3(p, q) \delta(q-q) \right) = \sigma_0 F_0 A_1 \left[ \sigma_0 F_0 (q-q) \right]. \quad (2.95)$$

With this association we no longer obtain a delta function along the $q=q_1$ line but rather an Airy function.

Let us now find $f_3(p, q)$ for a state given by the wave function specified by Eq. (2.76), an eigenstate of a particle of mass $m$ exposed to a constant force $F$, with energy $E$. This is given by

$$f_3(p, q) = \frac{\sigma_0 F_0}{\sigma_0 F_0 + \frac{3}{3} \sigma_3 F_3^{3/3}} \left[ \frac{\sigma_0 F_0}{\sigma_0 F_0 + \frac{3}{3} \sigma_3 F_3^{3/3}} \left( \frac{p^2}{2m} - Fq - E \right) \right]. \quad (2.96)$$

where $\sigma_0 F_0 = \sigma F$ this reduces to

$$f_3(p, q) = \delta \left( \frac{p^2}{2m} - Fq - E \right). \quad (2.97)$$

Thus, the $\hat{\Delta}_3(p, q)$ basis associates such $\delta$ functions with physically realizable states which are singular on parabolae (and not on straight lines) in the $p-q$ plane. Consequently, the association of $\delta$ functions which are singular on straight lines with physically realizable states was a special property of Wigner's function due to the special choice of basis [the latter being $\hat{\Delta}(p, q)$].

**Summary:** The image functions, $f(p, q)$, associated with the density matrix through different bases have widely different properties. For
the Wigner basis it is always real while for the Kirkwood basis it may be complex. With the Wigner basis it will be a delta function if and only if the delta function peaks along a straight line in the \( p,q \) space. Otherwise it will have a width proportional to \( \frac{\hbar^2}{3} \). For the Kirkwood basis, \( f(p,q) \) can only be a delta function of the delta function peaks along straight lines parallel to the \( p \) or \( q \) axis. It is possible to construct bases where it is a delta function for other curves, eg. parabola, or is never a delta function (normal ordering).

2.6 Expectation values

With the wide variety of possible associations it may be wondered how physical properties such as expectation values come out the same. In this section we will address that problem.

Quantum mechanically, the expectation value corresponding to a Hermitian operator \( \hat{A} \) is given by the trace:

\[
\langle \hat{A} \rangle \equiv \text{Tr}(\hat{A}) .
\]

If we have a basis \( \Delta_{\uparrow}^{\uparrow}(p,q) \) and an inverse basis \( \Delta_{\downarrow}^{\downarrow}(p,q) \) then we can write (see Eq. 2.6)

\[
\langle \hat{A} \rangle = \int d^3p d^3q f_{\uparrow}^{\dagger}(p,q) \Delta_{\uparrow}^{\uparrow}(p,q)/(2\pi\hbar)^3
\]

(2.99)

with a similar result for \( \Delta_{\downarrow}^{\downarrow}(p,q) \). Equation (2.99) is easily verified by substituting Eq. (2.100) into (2.98). For a basis such as the Wigner basis, \( \Delta(p,q) \) where the direct and inverse bases are the same, Eq. (2.99) is just a phase space integral as in the classical case. However, when we use a basis such as the Kirkwood basis, \( \Delta_{\uparrow}^{\uparrow}(p,q) \), where the direct and inverse bases are different we no longer have just an ordinary phase space integral since one of the
factors in the integrand comes from the direct basis while the other comes from the inverse basis.

The spatial density case is obtained from Eq. (2.98) by taking

\[ \hat{A} = \delta(q-q') \]  \hspace{1cm} (2.101)

Since the function associated with this delta function through either the Wigner or Kirkwood \( \hat{A}(p,q) \) is again a delta function we have for the spatial density in these bases

\[ \rho(q) = \int d^3p \frac{f(p,q)}{(2\pi\hbar)^3} . \]  \hspace{1cm} (2.102)

This, however, is not true of the \( \hat{A}_3(p,q) \) basis defined in Eq. (2.93). There the image associated with the delta function of Eq. (2.101) is an Airy function. Thus we have

\[ \rho(q) = \int d^3p d^3q' f_3(p,q') \alpha_0 F_0 Ai[\alpha_0 F_0(q_1-q)]/(2\pi\hbar)^3 \]  \hspace{1cm} (2.103)

and the density is no longer obtained by a simple integration over \( p \). (However, it reduces to that in the classical limit.) Again we see special (and usually desirable) properties connected with the Wigner basis.

Summary: The expressions for expectation values vary somewhat from basis to basis. For the Wigner basis the expectation value is just the phase space integral of the product of the functions associated with the density matrix and the operator whose expectation value we want. The Kirkwood basis gives a more complicated result, again we have the phase space integral of a product but this time one factor is obtained with the direct basis while the other is obtained with the inverse basis. With both the Wigner and Kirkwood basis the spatial density is obtained by integrating the image of density matrix over \( p \). This is not true for more general basis.
2.7 Partial associations

Until now we considered only systems where the Hamiltonian was a function of p and q only. However, other degrees of freedom may also be present, for example the spin or isotopic spin. These have no classical limit (as long as we do not allow the spin to take an infinite number of values) and for this reason it is not useful to subject these operators to a similar treatment. However, what we can do is the following.

Consider, for example, a non-relativistic electron described by the Pauli equation (Balazs, Pauli 1976). The density operator in the x representation will be a matrix \( \langle x' | \hat{\alpha} \beta | x \rangle \), where \( \alpha, \beta \) are spin indices. We may subject the \( x, x' \) indices to a transformation and introduce \( f_{\alpha \beta}(p, q) \) where \( p, q \) are the variables in the W space. Thus we associate a matrix with each point \( p, q \). The same can, of course be done on the Dirac electrons; then the range of \( \alpha, \beta \) is from 1 to 4. (See deGroot 1974.)

In general we may introduce partial W transformations, attacking those \( \hat{p}, \hat{q} \) operators in which we expect the classical limit to be a good approximation. Consider for example a diatomic molecule. The nuclei will move nearly classically while the electrons will not. Let

\[ \langle x_1, x_2; x_1, \ldots, x_N | \hat{p} | x_1', x_2'; x_1', \ldots, x_N' \rangle \]

be the density matrix in the x representation. \( x_1, x_2 \) are the coordinates of the nuclei, \( x_1, \ldots, x_N \) those of the N electrons. Transforming on the \( x_1, x_2 \) variables we can introduce

\[ \langle x_1, \ldots, x_N | f(P_1, Q_1; P_2, Q_2) | x_1', \ldots, x_N' \rangle \]

an object which describes the motion of the nuclei in the W space, coordinated by \( P_1, Q_1, P_2, Q_2 \) while the electrons are still described by a density matrix in which \( P_1, Q_1, P_2, Q_2 \) appear parametrically. This appears to us as a natural
description for the use of the Born-Oppenheimer approximation (Balazs 1958; for the description of collective degrees of freedom in nuclei see Gross 1980).

Summary: It is possible to do partial transformations, transforming those $\hat{p}, \hat{q}$ operators in which we expect the classical limit to a good approximation while treating the remaining $\hat{p}, \hat{q}$ operators explicitly as operators. This is a natural description for the use of the Born-Oppenheimer approximation. Operators which act in spin as well coordinate space can also be handled by transforming the orbital parts and leaving the spin parts. Thus we associate a spin matrix with each point in the p,q space.

2.8 Mock phase-spaces

Let us review briefly the p,q manifolds we have studied. The classical p,q manifold, the 6N dimensional phase space is parametrized by the classical coordinates $q_1, \ldots, q_N$ and the associated canonical momenta $p_1, \ldots, p_N$. It is said to be invariant under canonical transformations because these leave the canonical equations of motion unchanged. This invariance property determines its geometrical structure. The manifold is not metric, the separation between two points has no invariant meaning.

Each association introduces a p,q manifold through the choice of a particular basis set, a mock phase-space for each association. The p,q labels simply enumerate the members of the set and in the usual applications one does not envisage any changes in these labels; the transformation properties of p and q are as yet undetermined, and without transformation rules there is no invariance and no geometrical structure. The operator algebra of quantum mechanics is invariant under
unitary transformations. The putative transformation rules for p,q in a given association must be of such nature as to allow a similar invariance of the relations among the images which correspond to the operator relations. This is hampered by the fact that associations provide non-local relations among the image functions. For this reason the action of a unitary transformation cannot be expressed as a relabeling of the points in the mock phase-space (Balazs 1980, 1981). Hence one needs additional guiding principles to invent p,q transformation and such has been provided by Balazs and Jennings (1983).

The relations between images in the p,q space generated by the Wigner association, are invariant under linear inhomogenous transformations. This leads naturally to a metric, albeit not a Riemannian one but an affine one (Balazs 1980, see also section 3.2).

However, there are differences in these mock phase-spaces which can be observed without the use of the transformation properties of the p,q labels. The properties responsible for these differences can in fact be utilised to understand what properties the transformations of the p,q labels should possess. A useful approach is to specify the differences in the image $f_B(p,q)$ of the density operator engendered by a particular basis. These properties were discussed in sections 2.5 and 2.6. They relate in particular to the following: a) is the image real or complex, b) can it be a delta function for a physically realisable state. c) if it can be a delta function what is the argument of the delta function, d) how does one construct expectation values given the image of the density operator and the image of the operator whose expectation value we seek, d) in particular if this operator is $\delta(p-p')$
or \( \delta(q-q) \), do we obtain this expectation value by a simple integration of \( f_{\beta}(p,q) \) over the other variable.

Summary: There are as many mock phase-spaces as operator bases \( \hat{\beta}(p,q) \). These spaces have a priori no geometrical structure, but it is possible and useful to endow with such. (The space in which Wigner's function is displayed turns out to be a metric space, but a non-Riemannian one.) The image of the density operator has different properties in each mock phase-space which can also be used to characterise the properties of this space.

3. Approximations to Wigner's Function and Kirkwood's Function

3.1 Wigner-Kirkwood expansion

It was pointed out in the last section that both the Wigner and Kirkwood representations of the projection operator of an energy eigenstate reduce in the classical limit to a delta function on the curve \( H(p,q) = E \). In this section we will present an expansion which has as the leading term a delta function and derivatives of delta functions for corrections terms. Such an expansion is possible despite the fact that in the Kirkwood representation, and to a lesser extent in the Wigner representation, this reduction to a delta function takes place through infinitely rapid oscillations and not through the peaking of the absolute value of the function. Questions about the validity and usefulness of the delta function expansions, which are complicated by the rapid oscillations, will be discussed later.

More than one method exists for doing the delta function expansion. For example one can work directly with the Wigner representation in the energy space as done by Voros and collaborators (Voros 1977; Grammaticos & Voros 1979), or one can work with the Laplace transform
(moment generating function) of the Kirkwood representation as done by Bhaduri and collaborators (Jennings, Bhaduri & Brack 1975; Jennings 1976). Related work has also been done by Kirzhnits 1957, 1967 and Hodges 1973. The choice of method is purely one of taste and computational ease. We shall use the method based on the Laplace transform of the Kirkwood representation and then argue that the other methods are equivalent.

We start with the quantum mechanical projection operator

$$\hat{P}(E) = \delta(E-\hat{H})$$

and its Laplace transform

$$\hat{Z}(\beta) = e^{-\beta \hat{H}}$$

The method consists of setting up a differential equation for \(\hat{Z}(\beta)\) or more precisely for the Kirkwood transform of \(\hat{Z}(\beta)\). To do this we differentiate \(\hat{Z}(\beta)\) with respect to \(\beta\) to obtain

$$\frac{\partial \hat{Z}(\beta)}{\partial \beta} = -\hat{H} e^{-\beta \hat{H}} = -\hat{H} \hat{Z}(\beta)$$

and then take the Kirkwood transform of this equation

$$\frac{\partial Z_K^{(\beta)}}{\partial \beta} = -\left[ -\frac{\hat{H}^2}{2m} V^2 - 1h \frac{p \cdot V}{m} + \frac{p^2}{2m} + V(q) \right] Z_K^{(\beta)}$$

where \(Z_K^{(\beta)}= (2\pi)^3 \langle x=q | Z(\beta) | k=p/\hbar \rangle \langle k=p/\hbar | q=x \rangle\) is the Kirkwood transform of \(\hat{Z}(\beta)\). To obtain Eq. (3.4) we have used the composition rule for the Kirkwood transformation and have assumed that the Hamiltonian is of the form

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

More general Hamiltonians can, in principle, be easily included but this tends to obscure the procedure through pure tedium. Equation (3.4) is a differential equation of second order because the Hamiltonian is quadratic in \(p\). If the Hamiltonian had higher powers in \(p\), then the order of the differential equation would have been higher. If we
had taken the Kirkwood transform of $\hat{Z}(\beta)\hat{A}$ rather than $\hat{A}\hat{Z}(\beta)$ we would not have obtained a differential equation of finite order but an integral equation. This illustrates the advantage one can make of the intrinsic asymmetry of the Kirkwood transformation. If we had used the Wigner transform instead, the equation obtained would have been very similar regardless of the order of $\hat{A}$ and $\hat{Z}(\beta)$, and for both orders would have yielded an integral equation (or a differential operator of infinite order). More will be said on the Wigner transform of Eq. (3.3) later.

To solve Eq. (3.4) approximately we try a solution of the form

$$Z_K(\beta) = e^{-\beta(p^2/2m+V(q))} \left[ 1 + \hat{w}_1(p,q,\beta) + \beta^2 \hat{w}_2(p,q,\beta) + \ldots \right] \tag{3.6}$$

(where we have written simply $q$ for $x-q$, and $p$ for $\frac{h}{\hbar}k$). Substituting this form for $Z_K(\beta)$ into Eq. (3.4) and equating equal powers of $\hbar$ we can obtain a recursion relation for the $w$'s. Thus we have

$$\frac{\partial w_n}{\partial \beta} = -\left[ \frac{1}{(\beta/m)(p\cdot W)} - \frac{1}{(l/m)p\cdot V} \right]w_{n+1} + \frac{1}{2m} \left[ \beta^2(W)^2 - V^2 - 2B(V^2)V \right]w_n - 2 \cdot \tag{3.7}$$

This can be solved recursively using the initial data $w_0=1$ and $w_{-1}=0$.

The first two nontrivial $w$'s are

$$w_1 = -\frac{1}{(\beta/m)p\cdot W} \cdot \tag{3.8}$$

$$w_2 = -\frac{1}{(\beta^2/4m)}V^2 + (\beta^3/6m)(W)^2 - (\beta^4/8m^2)(p\cdot W)^2 + (\beta^3/6m^2)(p\cdot V)^2 \cdot \tag{3.9}$$

The expressions for the higher order $w$'s are fairly lengthy but $w_3$ and $w_4$ can be found in Jennings 1976.

Laplace inverting equation (3.6) term by term we obtain [writing again $p$ and $q$ for $\frac{h}{\hbar}k$ and $x$, and $H(p,q)$ for $p^2/2m+V(q)$],
\[ \langle p | q \rangle \langle q | \delta(E-H) | p \rangle \equiv (\delta(E-H))_{K} = \]

\[ = \delta(E-H) - (\hbar/2m) (p \cdot \nabla) \delta''(E-H) + \]

\[ + \hbar^{2} \left\{ - \delta''(E-H) (\nabla^{2} / 4m) + \delta'''(E-H) (\nabla^{2})^{2} / 6m \right\} + p \cdot \nabla^{2} (E-H)(p \cdot \nabla) \]

\[ + \langle \nabla \rangle \delta(E-H)(p \cdot \nabla)^{2} \delta(E-H) + \delta(E-H) \left\{ (p \cdot \nabla)^{2} / 6m \right\} . \quad (3.10) \]

This result, then, is an expansion in terms of delta functions arranged in orders of \( \hbar \). There is no term proportional to the first derivative of a delta function. Such a term would act to shift the peak location.

It is a general feature of this expansion that all terms even in \( \hbar \) are real while all terms odd in \( \hbar \) are imaginary. The imaginary terms have arisen due to the lack of symmetry in the Kirkwood transformation. The terms odd in \( \hbar \), also being odd in \( p \), do not contribute to the density, which is then real, as it must be. Equation (3.10) has faults in common with other semi-classical expansions. For example the density obtained by integrating over \( p \) diverges at the classical turning points.

One can then ask: What use are Eqs. (3.6) through (3.10)? First of all, if we were interested in high temperature systems then Eqs. (3.6) through (3.9) would be directly usable and for smooth potentials (analytic on the real axis) and the series would be convergent for sufficiently high temperatures. The \( \hbar \) power series involves just a finite rearrangement of a power series in \( \beta \). An \( \hbar \) expansion is useful at high temperatures because we are averaging over many states and the fine details of the quantum mechanical states are averaged out. Any time we are interested in a system averaged over energy or phase space we expect the expansion given above to be useful. One example of such usefulness is in connection with Strutinsky smoothing (Jennings, Bhaduri & Brack 1975, see also Brack & Quentin 1981, Ring & Schuck 1980).
must be pointed out, however, that Eq. (3.10) is not suited for studying the details of individual quantum states.

Definition (3.1) implies that Eq. (3.10) is normalized so that the integral \( \int \delta(E-H)Kd^3p d^3q \) gives \( \hbar^3 \) times the density of states. This normalization is particularly convenient since the present expansion is often used to obtain the density of states. In the next section a different normalization will be used since there we will look at individual states by a different method.

Having \( \delta(E-H)_K \) we can now find the corresponding \( \hbar \) expansion for the Wigner transformed density \( \delta(E-H)_W \) by the use of the equation [see Eq. (2.45)]

\[
\delta(E-H)_W = e^{(i\hbar/2)(p \cdot q)} \delta(E-H)_K . \tag{3.11}
\]

Since \( \delta(E-H)_K \) is given as a series in powers of \( \hbar \), and we seek \( \delta(E-H)_W \) also as a power series in \( \hbar \), we expand the exponential in Eq. (3.11). To order \( \hbar^2 \) we have

\[
\delta(E-H)_W = \delta(E-H)+\hbar^2[-\delta''(E-H)V^2V/8m+\delta'''(E-H)[(V)^2/24m^2+
+p\cdot V)^2V/24m^2] . \tag{3.12}
\]

Equations (3.10) and (3.12) are equivalent in the sense that one can be obtained from the other in a finite number of steps using Eq. (3.11) or its inverse. In contrast to Eq. (3.10), Eq. (3.12) is real and has no odd powers in \( \hbar \).

We will now discuss alternative derivations of (3.12) which shed additional light on the nature of the \( \hbar \) expansion and are useful for actual calculations. Let us start by taking the Wigner transform of Eq. (3.3). This results in

\[
\frac{\partial Z_W(\beta)}{\partial \beta} = H_W(p,q)\exp\left\{ \frac{i\hbar}{2} (\hat{p} \cdot \hat{q} - \hat{q} \cdot \hat{p}) \right\} Z_W(\beta) , \tag{3.13}
\]
where \( \hat{V} \) acts to left, \( \hat{V} \) acts to the right. Since we want an \( \hbar \) expansion the exponential can be expanded formally in a Taylor series. Equation (3.13) is then solved by the same procedure as Eq. (3.4): that is, we substitute Eq. (3.6) into Eq. (3.13) and equate equal powers of \( \hbar \). The \( \mathbf{w}'s \) are different than in the previous case but we can again do the Laplace inversion to obtain (3.12). These two methods will give identical results order by order in \( \hbar \). This can be shown directly by working with the truncated versions of

\[
\exp(i\hbar/2)(\hat{V}_{\mathbf{q}} \cdot \hat{V}_{\mathbf{p}} - \hat{V}_{\mathbf{q}} \cdot \hat{V}_{\mathbf{p}}) \quad \text{and} \quad \exp(i\hbar/2)\hat{V}_{\mathbf{q}} \cdot \hat{V}_{\mathbf{q}}.
\]

A third method of obtaining a semiclassical expansion of \( \delta(E-H) \) was developed by Voros 1977, and used extensively (Grammaticos & Voros 1979) in connection with the shell correction method in nuclear physics and the energy density formalism. In this method we write \( \delta(E-H) \) as \( \delta(E-H-(H-H)) \) and expand it in powers of the operator \( (H-H) \). \( H(p,q) \) is a function of \( p \) and \( q \) (not \( x! \)) and thus commutes with \( H \). The idea is that \( H(p,q) \) can be so chosen that \( \text{Tr}\{(H-H)^n\hat{H}_W\} \) can be made a fast decreasing function of \( n \). We obtain

\[
\delta(E-H) = \delta(E-H) + (H-H)\delta'(E-H) + \frac{1}{2}(H-H)^2\delta''(E-H) + \ldots, \quad (3.14)
\]

or

\[
\delta(E-H)_W = \delta(E-H)+(H-W-H)\delta'(E-H)+\frac{1}{2}[(H^2)_W-2H_WH_W+H^2]\delta''(E-H) + \ldots \quad (3.15)
\]

We choose now \( H = H_W \). This choice makes the \( \delta' \) term vanish, and insures that \( \delta(E-H) \) is the only \( \hbar \) independent term. If the Hamiltonian is of the form

\[
\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(\hat{q})
\]

the coefficients of \( \delta'' \) and \( \delta''' \) contain all the \( \hbar^2 \) contribution. Hence to order \( \hbar^2 \) only these terms contribute. The odd powers in \( \hbar \) vanish due to the symmetry of Wigner's association. However, we note that the
ordering according to the order of the derivatives and according to the power of \( \hbar \) does not go hand in hand, and has to be reinvestigated if \( \hbar \) is of a different structure or we use a different association.

In fact it turns out that for the Kirkwood association choosing \( \mathcal{H} = \hbar \mathcal{X} \) retains terms linear in \( \hbar \) in the coefficient of \( \delta^\prime \), and the \( \hbar^2 \) dependence is now contained in the coefficients of \( \delta^\prime \prime \), \( \delta^\prime \prime \prime \) and \( \delta^\prime \prime \prime \prime \).

We may finally ask the following question. Given \( \delta(E-\hbar \mathcal{X})_H \) and \( \delta(E-\hbar \mathcal{X})_K \) up to and including \( \hbar^4 \) terms, are the two expansions consistent? They are related to each other by Eq. (2.45), which expresses the relation through an explicitly \( \hbar \)-dependent operation. If, however we substitute the two power series in \( \hbar \) into that equation and expand the operator to \( \hbar^4 \) we obtain an identity.

**Summary:** In the classical limit the function associated with the projection operator of an energy eigenstate reduces to a delta function on the curve \( \mathcal{H}(p,q) = E \). The corrections for finite \( \hbar \) can be obtained as a series involving derivatives of delta functions. Such an expansion is useful when we want quantities that are averaged over many quantum states.

### 3.2 Airy type approximations

In the previous sections we studied the images of an energy eigenstate as a formal power series in \( \hbar \). Since the convergence of this series, or its quality as an asymptotic series is open to doubt we may want to evaluate these functions using other types of approximations to gain a better qualitative understanding of the general form. We shall specialize to the study of Wigner's function, although others could be studied the same way.
The two approximations we shall study give results which are qualitatively similar and start with a similar idea. Obtain in the \( x \) representation an approximate expression for \( \psi_E(x) \), the eigenfunction belonging to the energy \( E \), and evaluate approximately the integral transformation leading to Wigner's function.

Balazs and Zipfel (1973) use the wavefunction in a uniform approximation valid everywhere including the turning points and the classically forbidden region. In the evaluation of the integral they expand the slowly varying arguments of rapidly varying function. The result valid near the \( H=E \) curve gives

\[
f(p,q) = \sigma(E,q) \approx 0.1 \left[ \sigma_0(H(p,q) - E) \right]^{2/3} / [\hbar k(q,E)]^{2/3}
\]

(3.17)

with

\[
\begin{align*}
S(q,E)/\hbar &= \int_q^{\alpha(E)} k(x,E) dx \\
k(x,E) &= \frac{1}{\hbar} \sqrt{2m(E-V(x))} \\
k(q,E) &= 0 .
\end{align*}
\]

(3.18)

We will analyse this result shortly. Berry (1977) uses WKB wave functions for the classically permitted region and does not evaluate Wigner's function outside that region. In evaluating the integral transform he uses a saddle point method which is applicable for coalescing saddle points. The saddle point approximation and symmetry considerations enable him to bypass the singularity generated by the classical turning point. His central result can be written in a very elegant manner for all points \( p,q \) for which \( H(p,q) < E \), \( E \) being the energy of the state studied.

\[
f(p,q) \sim \frac{1}{\sqrt{\pi}} \frac{1}{(\hbar^2 B)^{1/3}} \text{Ai} \left[ \frac{2}{(\hbar^2 B)^{1/3}} (I(p,q) - I(E)) \right].
\]

(3.19)

Here \( 2\pi I(p,q) \) = area inside that \( H \) equal constant curve on which the
point \( p, q \) lies. \( 2\pi I(E) \) is the area inside the \( H = E \) curve and

\[
B \equiv I^2_{pp} + I^2_{qq} - 2I_{pq} I_{qp}.
\] (3.20)

Here the subscripts denote derivatives evaluated at the point \( p, q \). In the limit \( \hbar \to 0 \), Eq. (3.19) reduces to

\[
f(p, q) \sim \frac{\delta(I(p,q) - I(E))}{(2\pi)}.
\] (3.21)

Due to the different normalization this differs from the leading term in Eq. (3.12) by a factor of the classical density of states \( (2\pi)\hbar/\partial I \).

The qualitative appearance of Wigner's function for a stationary state is as follows. The function has its maximum just inside the \( H = E \) curve; this maximum is confined to a ribbon of width \( \sim \hbar^{2/3} \). Outside this region the function declines through rapid oscillations on the concave side, and decays exponentially on the convex side. Deep in the interior of the classically forbidden region on the concave side further fine structured anomalies occur which, however, can be disregarded in practical applications. (For a generalisation of this for time dependent states see, Berry, Balazs 1979).

The appearance of the peculiar power \( \hbar^{1/3} \) \((\hbar^{1/3})^2 \) etc. in Wigner's function has a deep geometrical reason (Balazs 1980). We have observed already that Wigner's function of a realizable state can be only that of a \( \delta \) function if \( p, q \) appear linearly in its argument. Thus linear functions are distinguished over all others by the thinness of Wigner's function. This peculiarity of Wigner's function is produced by the fact that the basis \( \hat{\mathcal{A}} \) is invariant under linear inhomogeneous transformations of \( \hat{p}, \hat{q} \) and \( p, q \). Geometries which have this invariance property are affine geometries, and in geometries of this kind arc lengths and distances along normals can be specified; these distances are proportional to powers of an area to the one third power. The natural unit
for such an area is $\hbar$ hence the appearance of powers of $\hbar^{1/3}$. In fact, we can rewrite Berry's expression using quantities as affine arc lengths and affine normals (natural to this geometry) and find that the argument of the Airy function measures the normal distance from the $H=E$ curve according to the rules of affine geometry.

**Summary:** Wigner's function, $f(p,q)$, has a peak, with width of order $\hbar^{2/3}$, along the $H(p,q)=E$ curve when $\hbar$ is small but non-zero. On the convex side of the $H(p,q)=E$ curve, $f(p,q)$ decays exponentially, while on the concave side it oscillates. For points near $H(p,q)=E$ the Wigner's function can be written as an Airy function whose argument is proportional to a difference of two classical actions. The appearance of one third powers of $\hbar$ has deep geometrical significance related to invariance of the $\hat{\lambda}(p,q)$ basis under linear transformations.

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Appendix I.1: The Thomas-Fermi Variation

To perform the variation we express \( f_1 \) as \( f_1 = \theta(g(p,q)) \) where \( \theta(x) = 1 \) \( x > 0 \), \( \theta(x) = 0 \) \( x < 0 \), and embed the surface \( g(p,q) = 0 \) in a family where \( g > 0 \) is inside the closed surface, and \( g < 0 \) is outside.

Then

\[
\begin{align*}
E[g] &= \int \left[ \frac{1}{2m} p^2 + V(q) \right] \theta(g) d^3 p d^3 q + \frac{1}{2} (1-1/N) \int U(q,q') \theta(g(p,q)) \theta(g(p',q')) d^3 p' d^3 q' d^3 p d^3 q, \\
N[g] &= \int \theta(g) d^3 p d^3 q.
\end{align*}
\]

Let us vary \( g \) by altering it by the amount \( Dg \) (we use \( Dg \) for the change to avoid the confusion with Dirac's \( \delta \)). Then \( D\theta = \delta(g) Dg \) and \( DE - \lambda DN = 0 \) implies that

\[
\int d^3 p d^3 q Dg(p,q) K(p,q) \delta(g) = 0,
\]

where

\[
K(p,q) = \frac{1}{2m} p^2 + V(q) + (1-1/N) \int U(q,q') \theta(g(p',q')) d^3 p' d^3 q' - \lambda.
\]

The variation vanishes for any value of \( Dg \), if

\[
K(p,q) \delta(g) = 0.
\]

Thus \( K(p,q) \) must vanish for all values of \( (p,q) \) for which \( g(p,q) = 0 \);

\[
K(p,q) = 0, \text{ if } g(p,q) = 0.
\]

In other words all \( p,q \) points which lie on the surface \( g = 0 \) must also lie on the \( K = 0 \) surface, or the \( g(p,q) = 0 \) surface must be part of the \( K(p,q) = 0 \), surface, or coincide with it altogether. (The \( g=0 \) surface must equal the \( K=0 \) surface or a portion of it. If it were the other way around \( K\delta(g) \) would not be zero on the excess \( g=0 \) surface.) Thus the boundary surface is given by part or the whole of the surface

\[
g = \frac{1}{2m} p^2 + U(q) - \lambda = 0
\]

with
\( U(q) = V(q) + (1 - 1/N) \int U(q,q') \delta(g(p',q')) d^3p' d^3q'. \)

Eliminating \( g \) we get an integral equation for \( U(q) \); \( \lambda \) is determined by the normalization condition.

For Coulomb forces the integral equation reduces to a differential equation. Let

\[ U(q) = -|e| \phi(q), \quad V(q) = -Ze^2/|q|, \quad \text{and} \quad u(q,q') = e^2/|q-q'|. \]

Since

\[ \frac{\Delta}{|q-q'|} = -4\pi \delta(q-q') \]

we obtain

\[ -|e| \Delta \phi = 4\pi \left[ Ze^2 \delta(q) - (1 - 1/N)e^2 \int \delta(g(q,p')) d^3p' \right] \]

or

\[ \Delta \phi = |e| n(q) - 4\pi |e| \delta(q), \]

(AII.1)

with

\[ n(q) = (1 - 1/n) \int \delta(g(q,p')) d^3p', \]

(AII.2)

where

\[ g = \frac{1}{2m} p^2 - |e| \phi - \lambda, \]

(AII.3)

and

\[ \int n(q) d^3q = N. \]

(AII.4)

The last four equations determine the three functions \( \phi, n, g \), and the constant \( \lambda \). They are the Thomas-Fermi equations.

Appendix II.I: The \( \hat{T} \) operator

In this appendix we give the properties of the \( \hat{T} \) bases. The operator \( \hat{T} \) is defined by

\[ \hat{T}(u,v) = \exp i(u \cdot \hat{r} + v \cdot \hat{q}) = e^{-(i\hbar/2)u \cdot v} e^{iu \cdot \hat{p}} e^{iv \cdot \hat{q}} = e^{+(i\hbar/2)u \cdot v} e^{iv \cdot \hat{q}} e^{iu \cdot \hat{p}} \]

(AII.1)

where \( u \) and \( v \) are real and \( u \cdot p = u_x \rho^x + u_y \rho^y + u_z \rho_z \). Probably the most important relation is the duplication formula
\[
\hat{T}(u,v)\hat{T}(u',v') = e^{(i\hbar/2)(u'v' - v'u')}\hat{T}(u+u', v+v')
\]

\[
= \exp(i\hbar D_2/2)\hat{T}(u+u', v+v')
\]

(AII.2)

\[
D_2 = \begin{vmatrix}
\hat{u}' & \hat{v}' \\
\hat{v}' & \hat{u}'
\end{vmatrix} = \hat{u}' \hat{v}' - \hat{v}' \hat{u}'
\]

(AII.3)

The duplication formula and the alternate forms in Eq. (AII.2) follow from the relation

\[
e^\hat{A} e^\hat{B} = e^{\hat{A}\hat{B}+(1/2)[\hat{A},\hat{B}]}
\]

(AII.4)

which is valid when \( \hat{A} \) and \( \hat{B} \) commute with their commutator. From the above relation we get the following results

\[
\hat{T}(u,v)\hat{T}(-u,-v) = \hat{T}(0,0) = 1
\]

(AII.5)

or

\[
\hat{T}^{-1}(u,v) = \hat{T}(-u,-v)
\]

\[
[\hat{T}(u,v),\hat{T}(u',v')] = 2i \sin(\frac{\hbar}{2} D_2)\hat{T}(u+u', v+v')
\]

(AII.6)

\[
\hat{T}(u,v)\hat{T}(u',v')\hat{T}(u'',v'') = e^{i\hbar/2D_3} \hat{T}(u+u'+u'', v+v'+v'')
\]

(AII.7)

\[
D_3 = \begin{vmatrix}
\hat{u} & \hat{v} & \hat{u}' & \hat{v}' & \hat{u}'' & \hat{v}''
\end{vmatrix}
\]

(AII.8)

In general we have

\[
T(u_0,v_0)T(u_1,v_1) \cdots T(u_N,v_N)T(u_{N+1},v_{N+1})
\]

\[
= \exp(i\hbar D_{N+1}/2)\hat{T}\left(\sum_{0}^{N} u_n, \sum_{0}^{N} v_n\right)
\]

(AII.9)

with

\[
D_{N+1} = \begin{vmatrix}
\sum_{0}^{N} u_n & \sum_{0}^{N} v_n \\
\sum_{1}^{N} u_n & \sum_{1}^{N} v_n
\end{vmatrix}
\]

(AII.10)

The above relations are useful in deriving the composition formulae for the image functions.

We now give the \( \hat{T} \) operator in different representations:

\[
\langle x' | \hat{T}(u,v) | x'' \rangle = \delta(x'-x''+hu) e^{iv(x'+x'')/2}
\]

(AII.11)

\[
\langle k' | \hat{T}(u,v) | k'' \rangle = \delta(-k'+k''+v) e^{ihu*(k'+k'')/2}
\]

(AII.12)
\( \langle k'|T(u,v)|x' \rangle = \frac{1}{(2\pi)^{3/2}} \exp \left[ -i \frac{u^* v + iv^*}{2} + \frac{i}{2} \right] \) \quad (AII1.13)

The states \( |x'\rangle \) and \( |k'\rangle \) are defined by

\[ \hat{p}|k'\rangle = \hat{\pi} k'|k'\rangle \quad (AII1.14) \]
\[ \hat{q}|x'\rangle = x'|x'\rangle \]

\[ \langle k'|k'' \rangle = \delta(k'-k'') \quad \langle x'|x'' \rangle = \delta(x'-x'') \] \quad (AII1.15)

As an example we derive Eq. AII1.11.

\[ \langle x'|T|x'' \rangle = \langle x'|\exp i(u\hat{p} + v\hat{q})|x'' \rangle \]
\[ = \langle x'|\exp i(v\hat{q})\exp i(u\hat{p})|x'' \rangle \exp \left( -\frac{iv^* u}{2} \right) \]
\[ = \langle x'|\exp i(u\hat{p})|k\rangle|d^3k\exp iv\hat{q}|x'' \rangle \exp \left( -\frac{iv^* u}{2} \right) \]
\[ = \left( \frac{2\pi}{4\theta} \right)^3 \delta(u-u') \delta(v-v') \]

The following trace relations can be derived using the above representations of \( \hat{T} \)

\[ \text{Tr}(\hat{T}(u,v)) = \left( \frac{2\pi}{4\theta} \right)^3 \delta(u) \delta(v) \] \quad (AII1.16)
\[ \text{Tr}[\hat{T}(u,v)\hat{T}(-u',-v')] = \text{Tr}[\hat{T}(u,v)\hat{T}^{-1}(u',v')] \]
\[ = \left( \frac{2\pi}{4\theta} \right)^3 \delta(u-u') \delta(v-v') \] \quad (AII1.17)

We can write an arbitrary operator \( \hat{A} \) in terms of the \( \hat{T} \) operators as

\[ \hat{A} = \int \tilde{A}(u,v)\hat{T}(u,v)d^3u d^3v \] \quad (AII1.18)

where \( \tilde{A}(u,v) \) is determined by

\[ \tilde{A}(u,v) = \left( \frac{2\pi}{4\theta} \right)^3 \text{Tr}[\hat{T}(-u,-v)\hat{A}(p,q)] \] \quad (AII1.19)

This last expression is verified by substituting for \( \hat{A} \) from Eq. (AII1.18) and using the duplication formula Eq. (AII.2) and the trace relation Eq. (AII.16). The following are simple examples

\[ \tilde{q} = \left( \frac{2\pi}{4\theta} \right)^3 \text{Tr}[\hat{T}(-u,-v)] = i \delta(u) \hat{v} \delta(v) \] \quad (AII1.20)
\[ \tilde{p} = \left( \frac{2\pi}{4\theta} \right)^3 \text{Tr}[\hat{T}(-u,-v)] = i \delta(v) \hat{u} \delta(u) \] \quad (AII1.21)
\[ (\tilde{q}\tilde{p}) = \left( \frac{2\pi}{4\theta} \right)^3 \text{Tr}[\hat{T}(-u,-v)] = -[(\hat{u} - i\mu u/2)\delta(v)] [(\hat{v} - i\mu v/2)\delta(u)] + 3i\mu/2 \delta(u) \delta(v) \] \quad (AII1.22)
Composition rules

\[ \tilde{C} = \hat{\Delta} \]

\[ \tilde{C}(u',v') = \int d^3\omega^3 \tilde{A}(u+u'/2, v+v'/2) \tilde{A}(u'/2-u, v'/2-v) \times \exp\left(\frac{i\hbar}{2}(v'\cdot u-u'\cdot v)\right) . \]

\[ \text{(AII1.23)} \]

Appendix II.2: The \( \hat{\Delta} \) operator

The operator \( \hat{\Delta} \) is defined by

\[ \hat{\Delta} = (\pi/2\hbar)^3 \int \delta(-u,-v) \exp i(u\cdot p+v\cdot q) d^3\omega^3 \nu . \]

\[ \text{(AII2.1)} \]

Hence the Fourier decomposition, \( \tilde{A}(u,v) \) is just

\[ \tilde{A}(u,v) = (\pi/2\hbar)^3 \exp[-i(u\cdot p+v\cdot q)] . \]

\[ \text{(AII2.2)} \]

The \( \hat{\Delta} \) operator has the following properties

\[ \int \Delta(p,q) d^3p d^3q = (2\pi\hbar)^3 \]

\[ \text{(AII2.3)} \]

\[ \text{Tr} (\hat{\Delta}(p,q) \hat{A}(p',q')) = (2\pi\hbar)^3 \delta(p-p') \delta(q-q') . \]

\[ \text{(AII2.5)} \]

These are consequences of the \( \hat{\nu} \) relations, (Appendix I.1).

\[ \hat{\Delta}(p,q) \hat{\Delta}(p',q') = \frac{4^3}{(2\pi\hbar)^3} \int d^3p'' d^3q'' \Delta(p'',q'') \exp\left(-\frac{2i}{\hbar}\begin{pmatrix} p & q \\ p' & q' \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix}\right) \]

\[ \hat{\Delta}(p,q) \hat{A}(p,q) = 4^3 \]

\[ \text{(AII2.6)} \]

or

\[ \Delta^{-1}(p,q) = \hat{\Delta}(p,q)/4^3 \]

\[ \langle x' | \Delta | x'' \rangle = \delta\left(\frac{x'+x''}{2} - q\right) e^{i(x'-x'')\cdot p/\hbar} \]

\[ \text{(AII2.9)} \]

\[ \langle k' | \Delta | k'' \rangle = \eta^3 \delta(p - \frac{(k'+k'')}{2}) e^{i q''(k''-k')} . \]

\[ \text{(AII2.10)} \]

The fundamental relations between the operators and image function are as follows,

\[ \hat{\Delta} = \int \frac{d^3p d^3q}{\hbar} A(p,q) \Delta(p,q) A(p,q) \]

\[ \text{(AII2.11)} \]

\[ A(p,q) = \text{Tr}(\Delta(p,q) \hat{\Delta}) . \]

\[ \text{(AII2.12)} \]

These are elementary consequences of the relations for the \( \hat{\nu} \) operators.

Note that we have
The composition rules are as follows:

For a product

$$\hat{C} = \hat{A} \hat{B}$$

(AII2.14)

$$C_w(p,q) = \frac{1}{(\pi \hbar)^6} \int d^3p' d^3q' d^3p'' d^3q'' \exp \left( - \frac{2i}{\hbar} \left| \begin{array}{l} p' q' \\ p'' q'' \end{array} \right| \right) \times$$

$$\times A_w(p', q') B_w(p'', q''),$$

(AII2.15)

$$= \exp \left\{ \left( \frac{i}{2} \right) \left( q' \cdot p' - q'' \cdot p'' \right) \right\} A_w(p, q) B_w(p, q),$$

(AII2.16)

$$= A_w(p, q) \exp \left( \frac{\hbar}{2} \right) B_w(p, q).$$

(AII2.17)

For the commutator

$$\hat{D} = -i[\hat{A}, \hat{B}]$$

(AII2.18)

$$D_w(p, q) = 2 \sin \left[ \frac{\hbar}{2} \left( q' \cdot p' - q'' \cdot p'' \right) \right] A_w(p, q) B_w(p, q),$$

(AII2.19)

An analogous set of results exists for the $\Delta_x$ basis and is listed below.

$$\hat{\Delta}_x^+ = \hbar \delta(p-q) \delta(q-q) = \langle \hbar / 2 \pi \rangle^3 \int (-u, -v) T(u, v) e^{+i(\hbar u + v)/2} d^3u d^3v$$

(AII2.20)

$$\hat{\Delta}_x^- = \hbar \delta(q-q) \delta(p-p) = \langle \hbar / 2 \pi \rangle^3 \int (-u, -v) T(u, v) e^{-i(\hbar u + v)/2} d^3u d^3v$$

(AII2.21)

$$\int \hat{\Delta}_x^+ d^3p d^3q = \int \hat{\Delta}_x^- d^3p d^3q = (2\pi \hbar)^3$$

(AII2.22)

$$\text{Tr} \hat{\Delta}_x^+ = \text{Tr} \hat{\Delta}_x^- = 1$$

(AII2.23)

$$\text{Tr} \hat{\Delta}_x^+ (p', q') \hat{\Delta}_x^- (p, q) = \hbar \delta(p-p') \delta(q-q'),$$

(AII2.24)

$$\text{Tr} \hat{\Delta}_x^+ (p, q) \hat{\Delta}_x^- (p', q') = \exp \left( -i(p-p') \cdot (q-q') / \hbar \right),$$

(AII2.25)

$$\text{Tr} \Delta_x^+(p, q) \Delta_x^-(p', q') = \exp \left( +i(p-p') \cdot (q-q') / \hbar \right),$$

$$\langle x | \hat{\Delta}_x^+(p', q') \rangle = \langle x' | \hat{\Delta}_x^- (p, q) \rangle = \delta(q-q') e^{i p' \cdot (x-x') / \hbar},$$

(AII2.26)

$$\hat{\Delta}_x^+(p, q) \hat{\Delta}_x^-(p', q') = \int d^3p d^3q - \delta(q-q') \delta(p-p') \exp \left( i(p-q') \cdot (p-p') / \hbar \right) \times$$

$$\times \hat{\Delta}_x^+(p, q),$$

(AII2.27)

$$\Delta_x^+(p, q) = \text{Tr} \left( \hat{\Delta}_x^+(p, q) \hat{\Lambda} \right), \Delta_x^-(p, q) = \text{Tr} \left( \hat{\Lambda} \hat{\Delta}_x^-(p, q) \right),$$

(AII2.28)

$$\hat{\Lambda} = \left( \langle k-p/\hbar | A | q \rangle \langle q | A^- | k-p/\hbar \rangle \right)^3 \int d^3p d^3q A_x^+(p, q) \Lambda_x^-(k, q)$$

(AII2.29)

$$\Delta_x^+(p, q) = (2\pi)^3 \langle k-p/\hbar | A | q \rangle \langle q | A^- | k-p/\hbar \rangle$$

(AII2.30)
Tr\left( \hat{A}_K(p,q)\hat{A}_K^{\dagger}(p',q') \right) = (1/\hbar)^3 \int d^3p' d^3q' \ A_k^+(p,q') B_k^+(p',q) \exp(i(p-p') \cdot (q-q')/\hbar) \\
= \exp(i\hbar \nabla_p \cdot \nabla q_1) A_k^+(p_1,q_1) B_k^+(p,q) \bigg|_{p_1=p, q_1=q} \hfill (AII2.31) \\
\hat{\delta} = -i[\hat{A}, \hat{B}] \hfill (AII2.32) \\
D_k^+(p,q) = -i\{\exp[i\hbar \nabla_p \cdot \nabla q_1] - \exp[i\hbar \nabla_p \cdot \nabla q_1]\} A_k^+(p_1,q_1) \times \hfill (AII2.33) \\
\times B_k^+(p,q) \bigg|_{p_1=p, q_1=q} \\
A_k^-(q,p) = (1/\hbar)^3 \int d^3p' d^3q' \exp(-i(p-p') \cdot (q-q')/\hbar) A_k^+(p',q') \\
= \exp(-i\hbar \nabla_p \cdot \nabla q_1) A_k^+(p,q) \hfill (AII2.34) \\
Relations between the \hat{A} and \hat{\delta}_K bases \\
Tr(\hat{A}(p,q)\hat{\delta}_K(p',q')) = 2\exp(2i(p-p') \cdot (q-q')/\hbar) \\
= \hbar^3 \exp\left(\frac{i\hbar}{2} \nabla_p \cdot \nabla q_1\right) \delta(p-p') \delta(q-q') \hfill (AII2.35) \\
\Lambda_k(p,q) = (2/\hbar)^3 \int d^3p' d^3q' \exp(-2i(p-p') \cdot (q-q')/\hbar) A_k^+(p',q') \\
= \exp\left(-\frac{i\hbar}{2} \nabla_p \cdot \nabla q_1\right) A_k^+(p,q) \hfill (AII2.36) \\
\Lambda_k^+(p,q) = (2/\hbar)^3 \int d^3p' d^3q' \exp(2i(p-p') \cdot (q-q')/\hbar) A_k(p',q') \\
= \exp\left(\frac{i\hbar}{2} \nabla_p \cdot \nabla q_1\right) A_k(p,q) \hfill (AII2.37) \\
\Lambda_k = \int d^3u^3v^3 \tilde{\Lambda}(u,v) \exp(i\hbar(u^*p + v^*q)) \hfill (AII2.38) \\
\Lambda_k^+ = \int d^3u^3v^3 \Lambda(u,v) \exp(-i\hbar(u^*p + v^*q)) \exp(-\frac{i\hbar u^*v}{2}) \hfill (AII2.39) \\
Appendix II.3 \\
A further insight can be obtained into the properties of Wigner's function, if we write out the density operator associated with the WKB wave function $\langle x' | = C \exp(i S(x',E)/\hbar - iEt/\hbar, E = \sqrt{2mE-V(x')} dx'$ and $V(x)$ varies very slowly with $x$. \\
Then $E = V(x_t)$ defines a turning point. Then \\
$\langle x' | p_1 | x'' \rangle \sim \frac{1}{\sqrt{k(x)k(x')}} \exp\left[\frac{i}{\hbar}(S(x') - S(x''))\right] \hfill (AII3.1) \\
Put now $x' = q-z/2, x'' = q+z/2$, and expand to lowest order in $z$. Then \\
$\langle x' | p_1 | x'' \rangle \sim \frac{1}{k(q)} \exp\left[ik(q)z\right] = g(q,z) \hfill (AII3.2)
The transformation from $x', x''$ to $q$ and $z$ corresponds to a $45^\circ$ rotation of the axes; hence $q = (x' + x'')/2$ labels a matrix element according to its location along the diagonal, and $z$ its perpendicular distance from the diagonal. The diagonal elements are proportional to $k^{-1}$; or to the reciprocal velocity, or to the classical sojourn time at $q$. This is indeed proportional to the probability of the particle being at $x$ in the element $dx$. Let us look now at the imaginary part of the matrix which is proportional to $(\sin kz)/k$. Its first zero will be for $k(q)z = \pm \pi$ or $z = \pm \pi/k(q) = \pi/2(hk)$. These define two slowly undulating curves lying symmetrically along the diagonal, the $q$ axis. The distance between these curves is just the local de Broglie wavelength. Conversely, knowing the oscillations of $g(q,p)$ in $z$, keeping $q$ fixed, gives one, through de Broglie's relation, the local classical momentum $\sqrt{2m(E-V(q))}$ in the region where the semi-classical approximation holds. The wavelength of these undulations in $z$ can formally be extracted by a Fourier transformation in the $z$ variable, giving

$$f(q,p) = \int g(q,z)e^{-ipz/k}\frac{dz}{h} = \frac{1}{k(q)}\delta(k(q)-p), \quad (A113.3)$$

where the Fourier transformation tells the harmonic content of $g(q,z)$ corresponding to the wavelength $k/p$ in $z$.

The steps taken can be replaced by one operation

$$\langle dx' < x' | \beta | x'' > dx'' \delta\left(\frac{x''+x'}{2} - q\right)e^{-i(x''-x')}p/k \text{ or } Tr(\hat{\Delta}(p,q)). \quad (A113.4)$$

Thus we see that steps to reach Wigner's function can be viewed as an effort to give an intuitive meaning of the density operator as a joint distribution function in new variables $p$ and $q$ which already in the semiclassical regime have a meaning similar to coordinates and associated momenta, the latter being introduced by the basic de Broglie
relation. While this gives a satisfactory meaning to the variables, it does not give the meaning of a joint probability to \( f(p, q) \) because the latter is not positive definite. The lack of this property does not hinder the computation of averages as if it were a bona fide probability density; however, it stops us from using it to construct a conditional probability. For example if \( f_2(p, q; p_2, q_2) \) is Wigner's function associated with the pair of particles 1 and 2, and \( f_1(p_1, q_1) \) in Wigner's function obtained by interpreting \( f_2 \) over \( p_2, q_2 \), we cannot use the relation \( f_2(p_1, q_1; p_2, q_2) = F(p_1, q_1; p_2, q_2) f_1(p_2, q_2) \) to define a conditional probability \( F(p_1, q_1; p_2, q_2) \), since \( f_1 \) is not positive definite and we cannot divide with it to extract \( F \) from the defining relation. This analysis shows further why Wigner's function will in general also become negative.

Appendix II.4: Normal ordering

In this appendix we discuss image functions associated with a basis defined through normal ordering and show that image functions are identical to the so called Glauber, or coherent-state representation of an operator.

The basis \( T_N(u, v) \) can be found as follows. [For a more detailed discussion see Voros (1977)]. We start by defining the raising and lowering operators

\[
\hat{a}^+ = (\hbar/2)^{1/2}[(-i/2)^{1/2} + i(m\hbar \omega)^{-1/2}\hat{p}] \quad \text{(AII4.1)}
\]

\[
\hat{a} = (\hbar/2)^{1/2}[(-i/2)^{1/2} - i(m\hbar \omega)^{-1/2}\hat{p}] \quad \text{(AII4.2)}
\]

where \( \omega \) and \( m \) are fixed but arbitrary parameters. These two operators obey the commutation relation

\[
[S, \hat{a}^+] = \hbar . \quad \text{(AII4.3)}
\]

As with the W and Kirkwood association we start in the \( u, v \) space.
Consider the operator
\[
\hat{T}_N^{-}(u,v) = \exp \left( i(u^+ p + v^+ q) \right) \exp \left[ (-\hbar/4)(v^2/\omega + u^2/\omega) \right]
\]
\[
= \exp \left[ i(\hat{a}^+ w + \hat{a}^+ w^*) \right] \exp \left[ -i\hbar w^*/2 \right]
\]
\[
= \exp i\hbar w \exp (i\hbar w^*)
\]  \quad (AII4.4)

where \( w = (1/\sqrt{2}) [v/(\omega 1/2) - iu(\omega 1/2)] \), and \( w^* \) is its complex conjugate. Thus we have an operator which puts the \( a \)'s before the \( a^+ \)'s. Similarly we can define an operator
\[
\hat{T}_N^{+}(u,v) = \exp (i\hbar^+ w^*) \exp (i\hbar w)
\]
\[
= \exp i(u^+ p + v^+ q) \exp \left[ (\hbar/4)(v^2/\omega + u^2/\omega) \right]
\]  \quad (AII4.5)

which is the inverse of \( \hat{T}_N \) in the sense that
\[
\text{Tr} \hat{T}_N^{+}(u,v) \hat{T}_N^{-}(-u',-v') = (2\pi/\hbar)^3 \delta(u-u') \delta(v-v'). \quad (AII4.6)
\]

Hence we can consider \( \hat{T}_N^{-} \) as the normal ordered \( \hat{T} \) basis and \( \hat{T}_N^{+} \) as the inverse basis.

As with the other associations we Fourier transform these operators
\[
\hat{\Lambda}_N^{-}(p,q) = \int d^3 u d^3 v \exp \left[ -i(p^+ u + q^+ v) \right] \hat{T}_N^{-}(u,v) (\hbar/2\pi)^3 \quad (AII4.7)
\]
\[
\hat{\Lambda}_N^{+}(p,q) = \int d^3 v d^3 u \exp \left[ -i(p^+ u + q^+ v) \right] \hat{T}_N^{+}(u,v) (\hbar/2\pi)^3. \quad (AII4.8)
\]

While \( \hat{\Lambda}_N^{-}(p,q) \) is a well defined operator \( \hat{\Lambda}_N^{+}(p,q) \) exists only as a distribution and it is difficult to define its matrix elements except in a special basis such as the harmonic oscillator basis with an oscillator frequency \( \omega \). We can now define the associated functions
\[
A_N^{-}(p,q) = \text{Tr} (\hat{\Lambda}_N^{-}(p,q)). \quad (AII4.9)
\]

To the extent that \( \hat{\Lambda}_N^{+}(p,q) \) exists we can write
\[
\hat{\Lambda} = \frac{1}{\hbar^3} \int d^3 p d^3 q \hat{\Lambda}_N^{+}(p,q) A_N^{+}(p,q) . \quad (AII4.10)
\]

The coefficients \( A_N^{-}(p,q) \) are related to \( A_N^{-}(p,q) \) by
Note that this is just a convolution and follows immediately from the product in the Fourier transform, \( \hat{\tau}^{-1}_N \).

In the harmonic oscillator basis \( \hat{\tau}_N(p,q) \) can be written as

\[
\langle n'| \hat{\tau}_N(p,q)|n \rangle = \frac{1}{[lnn']^{1/2}} \left( \frac{a}{\sqrt{\hbar}} \right)^{n'} \left( \frac{a^*}{\sqrt{\hbar}} \right)^n \times \exp\left(\frac{-1}{\hbar\omega}(p^{2}/2m+\omega^{2}q^{2}/2)\right)
\]

(AII4.12)

where

\[
a = (\hbar/2)^{1/2}[(\omega/\hbar)^{1/2}q +i(\omega\hbar)^{-1/2}p],
\]

(AII4.13)

and similarly for \( a^* \). \( \hat{\tau}_N(p,q) \) can also be written as

\[
\hat{\tau}_N(p,q) = \langle \psi_{pq} | \psi_{pq} \rangle.
\]

(AII4.14)

This follows immediately from Eq. (AII4.11) or Eq. (AII4.12) where \( |\psi_{pq}\rangle \) is given by

\[
\hat{a}^+ |\psi_{pq}\rangle = (\hbar/2)^{1/2}[(\omega/\hbar)^{1/2}q +i(\omega\hbar)^{-1/2}p] |\psi_{pq}\rangle.
\]

(AII4.15)

Thus we have

\[
\hat{\tau}_N(p,q) = \langle \psi_{pq} | \hat{a}^+ |\psi_{pq}\rangle.
\]

(AII4.16)

From this form of \( \hat{\tau}_N(p,q) \) we see that \( \hat{\tau}_N(p,q) \) will be positive for all \( p \) and \( q \) if \( \hat{a} \) is a positive definite operator such as the density matrix. This desirable feature was not present with the \( W \) and Kirkwood associations.

The Wigner \( \hat{\tau}(p,q) \) and \( \hat{\tau}_N(p,q) \) are related by

\[
\text{Tr}(\hat{\tau}(p,q) \hat{\tau}_N(p',q')) = 2^3 \exp\left(\frac{-2}{\hbar\omega}\left[(p-p')^2/2m+\omega^2(q-q')^2/2\right]\right)
\]

(AII4.17)

so we also have

\[
A^+(p,q) = \int \frac{d^3p'd^3q'}{\hbar^3} A_N(p',q') 2^3 \exp\left(\frac{-2}{\hbar\omega}\left[(p-p')^2/2m+\omega^2(q-q')^2/2\right]\right).
\]

(AII4.18)

The right hand side of Eq. (AII3.16) is often called the Glauber or coherent state representation of the operator \( \hat{\tau} \), \( A_{\text{coh}}(p,q) \), and is
considered the object representing quantum mechanically, the classical
dynamical quantity associated with the operator \( \hat{A} \). We notice that the
coherent state representation is simply another choice of basis in the
operator space corresponding to normal ordering. In this sense it has
very little to do with coherent states, or harmonic oscillator states.
The latter served simply as a mathematical tool to express the new
operator basis in a particularly convenient representation.

Appendix II.5

Consider a particle of mass \( m \) in a constant force \( F \). Its
Hamiltonian is given by \( p^2/2m - Fq \), and the classical trajectory in the
\( p, q \) space is given by the parabola \( p^2/2m - Fq = E \). Quantum mechanically
the energy spectrum is continuous and the eigenfunctions are the Airy
functions \( \text{Ai}(\xi) \), with \( \xi = (x + E/F)(2mF/k^2)^{1/3} \). In the semiclassical
approximation these eigenfunctions are given as

\[
\psi_E(x) \sim |\xi|^{-1/4} \left[ \exp \left( \frac{2}{3} \xi^{3/2} + \frac{i\pi}{4} \right) - \exp \left( -\frac{2}{3} \xi^{3/2} - \frac{i\pi}{4} \right) \right] ; \quad (\text{AII5.1})
\]

and as

\[
\phi_E(k) \sim \exp \left( \frac{i}{\hbar F} \left( \frac{E}{m} k - \langle E \rangle k \right)^{3/6} \right) \quad (\text{AII5.2})
\]
in the momentum representation \( k \).

These functions are needed to express Kirkwood's function in a
semiclassical approximation, since \( f_k^+(p, q) \) is given as

\[
f_k^+(p, q) \sim e^{-ipq/\hbar} \psi(x=q) \phi(k=p) . \quad (\text{AII5.3})
\]

Substituting the wave functions in the \( x \) and \( k \) representation, and
replacing \( x \) with \( q \) and \( k \) with \( p/\hbar \), we obtain

\[
f_k^+(p, q) \sim |\xi|^{-1/4} \left( e^{+(1/\hbar)\alpha_1} - e^{-(1/\hbar)\alpha_2} \right) , \quad (\text{AII5.4})
\]

where the fast varying phases \( \alpha_1/\hbar \), \( \alpha_2/\hbar \) are given by

\[
\alpha_1 = -pq + (Ep - p^3/6m)/F + (2/3)\hbar \xi^{3/2} , \quad (\text{AII5.5})
\]
\[
\alpha_2 = -pq + (Ep - p^3/6m)/F - (2/3)\hbar \xi^{3/2} . \quad (\text{AII5.6})
\]
The points on which phase $\alpha_1$ is stationary are given by the roots of the equations
\[ \frac{\partial \alpha_1}{\partial p} = -q + \frac{E}{F} - p^2/2mF = 0; \quad \frac{\partial \alpha_1}{\partial q} = -p + \xi^{1/2}(2mF)^{1/3} = 0; \quad \text{(AII5.7)} \]
and the points on which the phase $\alpha_2$ is stationary are given by the roots of the equations
\[ \frac{\partial \alpha_2}{\partial p} = -q + \frac{E}{F} - p^2/2mF = 0; \quad \frac{\partial \alpha_2}{\partial q} = -p - \xi^{1/2}(2mF)^{1/3} = 0. \quad \text{(AII5.8)} \]

Let us analyse the stationary points of $\alpha_1$. All points on the classical energy equation are solutions of the equation $\frac{\partial \alpha_1}{\partial p} = 0$. Of these, the second equation admits only those for which the value of the parameter $p$ is positive. Thus, for positive values of $p$ the stationary points of $\alpha_1$ lie on the positive momentum branch of the classical energy equation; if $p$ is negative, $\alpha_1$ has no stationary points. Similarly, the stationary points of $\alpha_2$ lie on the negative $p$ branch of the classical energy curve, and $\alpha_2$ has no stationary points for positive values of $p$. Consequently, there are always stationary points for the phase of $f(q,p)$, and they always lie on the classical energy curve. It is revealing to analyse this problem in more geometrical terms showing that the classical energy equation specifies that curve in the $p,q$ space on which the two waves $\Psi(q)$ and $\Phi(p)e^{-ipq/\hbar}$ interfere. Consider for example the phase $\alpha_1(p,q)$. This contains two additive contributions, $(2/3)\xi^{3/2}$ from the $\Psi$ wave and $-pq+(E-p^3/6m)$ $F$ from the $\Phi(p)e^{-ipq/\hbar}$ wave. At the stationary points the gradient of the sum must vanish, hence the gradient of the two terms must be parallel to each other, or the curves of constant phase of each wave must be parallel to each other; they must touch. The surfaces of constant phase of the $\Psi(q)$ wave are represented by lines parallel to the $p$ axis, the surfaces of the other wave are given by the equation $-pq+(E-p^3/6m)/F=C$. 
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