## Evolution of moments over quantum wavepackets or classical clusters

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# Evolution of moments over quantum wavepackets or classical clusters 

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#### Abstract

Using a symplectic notation which allows the equations to apply equally to a wavepacket representing a spin-less quantum particle or to a cluster of identical classical particles without mutual interactions, the study of the time-evolution of moments is extended to arbitrary orders for arbitrary Hamiltonians. Appropriately symmetrised moments for the quantum case are seen to play a special role and correspond very closely to the classical moments.


## 1. Introduction

The evolution in time of the state of a quantum system can be represented, at least formally, by the evolution of the moments over the system. This is most appropriate for a wavepacket, i.e. a quantum state where the spread of position and momentum are in some sense small. Here the close parallels between classical and quantum mechanics will be exploited to deal simultaneously with the evolution of moments over a quantum wavepacket and those over a classical system of particles without mutual interactions, again without a large spread in position or momentum values (i.e. a cluster). Moments are averages of products of deviations from some reference value of position and momentum. In the quantum case the average will be the usual expectation value over the wavepacket while in the classical case it will be the mean over the particles in the cluster.

Earlier work by Messiah (1961), Andrews (1981a, b) and Reid and Ray (1983) has dealt with such systems where the motion is describable by a potential, by expanding the potential in series of powers of deviations from the reference trajectory. For the case of a classical cluster, this approach has been extended to motion under an arbitrary Hamiltonian (Andrews 1983). These papers gave approximate equations for the evolution of low-order moments where higher-order moments were neglected. Such an approximation scheme is valid where the wavepacket or cluster is sufficiently small on the scale of changes in the forces.

In what follows the quantum case will also be extended to an arbitrary Hamiltonian and both the quantum and classical cases will be extended to moments of arbitrary order.

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## 2. Notation

The symplectic notation (e.g. Goldstein 1980, Andrews 1983) will be used throughout. Thus Greek letters will run from 1 to $2 N$ where $N$ is the number of (generalised) coordinates required and $x^{\alpha}$ will represent both (generalised) position and momentum with $x^{i}, x^{i+N}(i=1,2, \ldots, N)$ denoting the $i$ th component of position and momentum respectively. The reference point for the evaluation of moments will be denoted by $\xi^{\alpha}$. In the quantum case $x^{\alpha}$ will be (a set of) operators but $\xi^{\alpha}$ will always be a $c$-number, that is it will commute with everything. The deviation from the reference trajectory will be $X^{\alpha}:=x^{\alpha}-\xi^{\alpha}$.

A typical moment is

$$
\begin{equation*}
\chi^{\alpha_{1} \ldots \alpha_{n}}:=\left\langle X^{\alpha_{1}} X^{\alpha_{2}} \ldots X^{\alpha_{n}}\right\rangle \tag{2.1}
\end{equation*}
$$

For a quantum system, the order of the $\alpha$ 's is important and the angled brackets denote the expectation value while for a classical system of $\mathcal{N}$ particles with the positionmomentum of the $A$ th particles denoted by $X_{A}^{\alpha}$,

$$
\begin{equation*}
\left\langle X^{\alpha_{1}} \ldots X^{\alpha_{n}}\right\rangle=\mathcal{N}^{-1} \sum_{A=1}^{\stackrel{\Downarrow}{x}} X_{A}^{\alpha_{1}} X_{A}^{\alpha_{2}} \ldots X_{A^{n}}^{\alpha_{n}} \tag{2.2}
\end{equation*}
$$

and the result is symmetric under interchange of any of the superscripts.

## 3. Exact equations for the evolution of the moments

Hamilton's classical equations of motion can be written

$$
\begin{equation*}
\dot{x}^{\alpha}=\varepsilon^{\alpha \beta} H_{\beta} \tag{3.1}
\end{equation*}
$$

where $H_{\beta}=\partial H / \partial x^{\beta}$ and $\varepsilon^{i, N+i}=1, \varepsilon^{N+i, i}=-1$ for $1 \leqslant i \leqslant N$ with all other elements of $\varepsilon^{\alpha \beta}$ zero. Differentiating (2.1), the time-derivative of the general moment for a classical cluster is

$$
\begin{align*}
& \dot{\chi}^{\alpha_{1} \ldots \alpha_{n}}=\sum_{i=1}^{n}\left\langle X^{\alpha_{1}} \ldots X^{\alpha_{i-1}} \dot{X}^{\alpha_{i}} X^{\alpha_{i+1}} \ldots X^{\alpha_{n}}\right\rangle \\
&=\sum_{i=1}^{n}\left\langle X^{\alpha_{1}} \ldots X^{\alpha_{i-1}}\left(\varepsilon^{\alpha_{i} \beta} H_{\beta}-\dot{\xi}^{\alpha_{i}}\right) X^{\alpha_{i+1}} \ldots X^{\alpha_{n}}\right\rangle \tag{3.2}
\end{align*}
$$

In the quantum case, the time-derivative of expectation values is obtained from

$$
\begin{equation*}
\mathrm{d}\langle A\rangle / \mathrm{d} t=\langle(\mathrm{i} / \hbar)[H, A]+\partial A / \partial t\rangle \tag{3.3}
\end{equation*}
$$

leading to

$$
\begin{aligned}
\dot{\chi}^{\alpha_{1} \ldots \alpha_{n}}=\left\langle\frac{i}{\hbar}\right. & {\left.\left[H, X^{\alpha_{1}} \ldots X^{\alpha_{n}}\right]+\frac{\partial}{\partial t}\left(X^{\alpha_{1}} \ldots X^{\alpha_{n}}\right)\right\rangle } \\
& =\sum_{i=1}^{n}\left\langle\frac{\mathrm{i}}{\hbar} X^{\alpha_{1}} \ldots X^{\alpha_{i-1}}\left[H, X^{\alpha_{i}}\right] X^{\alpha_{i+1}} \ldots X^{\alpha_{n}}-X^{\alpha_{1}} \ldots X^{\alpha_{i-1}} \dot{\xi}^{\alpha_{i}} X^{\alpha_{i+1}} \ldots X^{\alpha_{n}}\right\rangle
\end{aligned}
$$

The commutator can be evaluated with

$$
\begin{equation*}
\left[H, x^{\alpha}\right]=-\mathrm{i} \hbar \varepsilon^{\alpha \beta} H_{\beta} \tag{3.4}
\end{equation*}
$$

and hence both the classical and quantum cases can be written as
$\dot{\chi}^{\alpha_{1} \ldots \alpha_{n}}=\sum_{i=1}^{n}\left(\varepsilon^{\alpha_{i} \beta}\left(X^{\alpha_{1}} \ldots X^{\alpha_{i-1}} H_{\beta} X^{\alpha_{1+1}} \ldots X^{\left.\alpha_{n}\right\rangle}\right\rangle-\dot{\xi}^{\alpha_{i}} \chi^{\alpha_{1} \ldots \alpha_{1-1} \alpha_{i+1} \ldots \alpha_{n}}\right)$.
This equation of motion for the moments can be regarded as a generalisation of Ehrenfest's relation

$$
\begin{equation*}
\mathrm{d}\left\langle x^{\alpha}\right\rangle / \mathrm{d} t=\varepsilon^{\alpha \beta}\left\langle H_{\beta}\right\rangle, \tag{3.6}
\end{equation*}
$$

obtained from (3.5) by taking $n=1$ and $\xi^{\alpha}=0$.

## 4. Series expansion of the Hamiltonian

The evolution equations (3.5) are now converted into a set involving only moments by expanding $H_{\beta}$ about the reference trajectory $\xi^{\alpha}$, that is in powers of $X^{\alpha}$. Such Taylor expansion of an operator function has been discussed in the accompanying paper by Hall (1985). In general, the specification of an appropriate set of Taylor coefficients is complicated by the ambiguity in ordering the operators in the expansion.

Usually one is concerned with Hamiltonians which are symmetric in the sense used by Hall (1985, §5). Application of Weyl's rule to find the quantum Hamiltonian corresponding to a given classical Hamiltonian will always give a symmetric result. There exist operators which are Hermitian but not symmetric and we can see no good reason to exclude these as potential Hamiltonians, but as far as we know none has ever been proposed as physically realistic. For symmetric Hamiltonians one has available the simple result that the expansion can be expressed in terms of symmetric multinomials and then the coefficients are identical with those of the expansion of the corresponding classical Hamiltonian.

In any case one can write

$$
\begin{equation*}
H(x)=\sum_{k=0}^{\infty}(1 / k!) h_{\gamma_{1} \ldots \gamma_{k}} X^{\gamma_{1}} \ldots X^{\gamma_{k}} \tag{4.1}
\end{equation*}
$$

For a classical cluster,

$$
\begin{equation*}
h_{\gamma_{1} \ldots \gamma_{k}}=\left.\frac{\partial H(x)}{\partial x^{\gamma_{1}} \ldots \partial x^{\gamma_{k}}}\right|_{x=\xi} \tag{4.2}
\end{equation*}
$$

which is obviously symmetric. For a symmetric quantum Hamiltonian the $h_{\gamma_{1} \ldots \gamma_{k}}$ will also be symmetric and equal to those of the corresponding classical Hamiltonian; more generally they will be non-symmetric but their symmetrical part $h_{\left(y_{1} \ldots y_{k}\right)}$ will equal the coefficients of the corresponding classical Hamiltonian.

Inserting (4.1) into (3.5) and defining

$$
\begin{equation*}
\phi_{y_{1} \ldots \gamma_{k}}^{\alpha}:=[1 /(k+1)] \varepsilon^{\alpha \beta}\left(h_{\beta \gamma_{1} \ldots \gamma_{k}}+h_{\gamma_{1} \beta \gamma_{2} \ldots \gamma_{k}}+\ldots+h_{\gamma_{1}, \ldots \gamma_{k} \beta}\right) \tag{4.3}
\end{equation*}
$$

gives
$\dot{\chi}^{\alpha_{1} \ldots \alpha_{n}}=\sum_{i=1}^{n}\left\{\sum_{k=0}^{\infty}\left[(1 / k!) \phi_{\gamma_{1} \ldots \gamma_{k}}^{\alpha_{i}} \chi^{\alpha_{1} \ldots \alpha_{i-1} \gamma_{1} \ldots \gamma_{k} \alpha_{1+1} \ldots \alpha_{n}}\right]-\dot{\xi}^{\alpha_{1}} \chi^{\alpha_{1} \ldots \alpha_{i-1} \alpha_{i+1} \ldots \alpha_{n}}\right\}$.
This expresses the time-derivative of any moment in terms of all the moments and the coefficients of the Hamiltonian along the reference trajectory. Two important cases
for the choice of reference trajectory are the centroid $\left\langle x^{\alpha}\right\rangle$ and a solution of the corresponding classical equations of motion, $\dot{\xi}^{\alpha}=\varepsilon^{\alpha \beta} h_{\beta}=\phi^{\alpha}$. Such a solution with $\xi^{\alpha}(0)=\left.\left\langle x^{\alpha}\right\rangle\right|_{t=0}$ will be called the basal trajectory. The centroid is itself a moment (of the first order) and its evolution equation is a special case of (4.4), putting $m=1$ and $\xi^{\alpha}=0$. Therefore reference to the centroid (which will be considered in $\S 8$ ) requires more complex schemes of approximation than reference to the basal trajectory, where $\xi^{\alpha}$ can be determined in advance by classical methods.

In the case of reference to the basal trajectory, the moment equations become

$$
\begin{equation*}
\chi^{\alpha_{1} \ldots \alpha_{n}}=\sum_{i=1}^{n} \sum_{k=1}^{\infty}(1 / k!) \phi_{\gamma_{1} \ldots \gamma_{k}}^{\alpha_{k}} \chi^{\alpha_{1} \ldots \alpha_{1-1} \gamma_{1} \ldots \gamma_{k} \alpha_{i+1} \ldots \alpha_{n}} \tag{4.5}
\end{equation*}
$$

This equation is exact; it is, in effect, another representation of Schrödinger's equation for the time-evolution of states in the quantum case and of Hamilton's equations of motion in the case of a classical cluster. The question of convergence is important but is ignored here.

## 5. Approximate calculation of the moments

If the deviations from the basal trajectory remain sufficiently small, on a scale set by the coefficients of the Hamiltonian, then the contribution to the right-hand side of (4.5) by high-order moments will be negligible. By neglecting moments of order greater than $n+m$ one can calculate moments of order $n$ accurate to order $n+m$. Such accuracy will be denoted by a subscript $m$; thus

$$
\begin{equation*}
\chi_{m}^{\alpha_{1} \ldots \alpha_{n}}=\chi^{\alpha_{1} \ldots \alpha_{n}}+\mathrm{O}(n+m+1) . \tag{5.1}
\end{equation*}
$$

A sequential scheme of calculation can be carried out using

$$
\begin{equation*}
\dot{\chi}_{m}^{\alpha_{1} \ldots \alpha_{n}}=\sum_{i=1}^{n} \phi_{\gamma}^{\alpha_{i}} \chi_{m}^{\alpha_{1} \ldots \alpha_{1-1} \gamma \alpha_{i+1} \ldots \alpha_{n}}+f_{m}^{\alpha_{1}, \ldots \alpha_{n}} \tag{5.2}
\end{equation*}
$$

where

$$
\begin{equation*}
f_{m}^{\alpha_{1} \ldots \alpha_{n}}:=\sum_{i=1}^{n} \sum_{k=2}^{m+1} \frac{1}{k!} \phi_{\gamma_{1} \ldots \gamma_{k}}^{\alpha_{k}} \chi_{m-1-c_{k}}^{\alpha_{1}, \alpha_{i-1}} y_{1} \ldots \gamma_{k} \alpha_{i+1} \ldots \alpha_{m} \tag{5.3}
\end{equation*}
$$

where the $c_{k}$ are arbitrary apart from the constraint $c_{k} \leqslant k-2$. This differential equation is solved for $\chi_{m}^{\alpha_{1} \ldots \alpha_{n}}$ subject to the initial condition

$$
\begin{equation*}
\left.\chi_{m}^{\alpha_{1} \ldots \alpha_{n}}\right|_{t=0}=\left.\chi^{\alpha_{1} \ldots \alpha_{n}}\right|_{t=0} \tag{5.4}
\end{equation*}
$$

it being arranged that at every stage $f_{m}^{\alpha_{1} \ldots \alpha_{n}}$ is known as a function of time from earlier integrations in the sequence. The ambiguity represented by the arbitrary constants $c_{k}$ merely reflects the possibility of using, in $f_{m}^{\alpha_{1} \ldots \alpha_{n}}$, moments more accurate than required provided they are available from earlier integrations. Equation (5.2) greatly generalises equations (4.2) and (4.3) of Andrews (1983).

## 6. Symmetrised moments in terms of classical trajectories

In the case of symmetrised moments $\chi^{\left(\alpha_{1} \ldots \alpha_{n}\right)}$, which are averaged over all permutations of the indices, the differential equation for the time evolution will now be solved in
terms of appropriate classical trajectories. The non-symmetric moments can be expanded in terms of the symmetric ones using Hall's relation (1984, equation (4.3)) and taking expectation values.

If in (5.2) the term $\Sigma_{i} \phi_{\gamma}^{\alpha_{i}} \chi_{m}^{\alpha_{1} \ldots \alpha_{1-1} \gamma \alpha_{1+1} \ldots \alpha_{n}}$ is symmetrised over $\alpha_{1} \ldots \alpha_{n}$, the result is the same as $\Sigma_{i} \phi_{\gamma}^{\alpha} \chi_{m}^{\left(\alpha_{1}, \ldots \alpha_{i-1} \gamma \alpha_{1+1} \ldots \alpha_{n}\right) \text {. (This separability property does not extend to the }}$ terms in $f_{m}^{\alpha_{1} \ldots \alpha_{n}}$ and therefore it can be seen that even the symmetrical quantal moments do not have the same evolution as the corresponding classical moments. They do have the same evolution, however, when the Hamiltonian is quadratic.) Hence the symmetrised form of (5.2) is

$$
\begin{equation*}
\dot{\chi}_{m}^{\left(\alpha_{1} \ldots \alpha_{m}\right)}=\sum_{i=1}^{n} \phi_{\gamma}^{\alpha_{i}} \chi_{m}^{\left(\alpha_{1} \ldots \alpha_{i-1} \gamma \alpha_{i+1} \ldots \alpha_{n}\right)}+f_{m}^{\left(\alpha_{1} \ldots \alpha_{n}\right)} . \tag{6.1}
\end{equation*}
$$

This inhomogeneous differential equation for the moments of order $n$ can be solved, assuming $f_{m}^{\left(\alpha_{1}, \ldots \alpha_{n}\right)}$ is known as a function of time, by the method used in the classical case (Andrews 1983, §5). Thus let $u^{\alpha}{ }_{\beta}(t)$ be the solutions of $\dot{u}^{\alpha}{ }_{\beta}=\phi^{\alpha}{ }_{\gamma} u^{\gamma}{ }_{\beta}$ with $u^{\alpha}{ }_{\beta}(0)=\delta^{\alpha}{ }_{\beta}$. These can be found by differentiating the classical trajectories with respect to the initial position-momentum. Now define

$$
\begin{equation*}
G_{\beta}^{\alpha}\left(t, t^{\prime}\right)=u_{\gamma}^{\alpha}(t) \varepsilon^{\gamma \delta} u_{\delta}^{\sigma}\left(t^{\prime}\right) \varepsilon_{\sigma \beta}=u^{\alpha \gamma}(t) u_{\beta \gamma}\left(t^{\prime}\right) \tag{6.2}
\end{equation*}
$$

and the solution of (6.1) is

$$
\begin{align*}
& \chi_{m}^{\left(\alpha_{1} \ldots \alpha_{n}\right)}=\left.u_{\beta_{1}}^{\alpha_{1}} \ldots u_{\beta_{n}}^{\alpha_{n}} \chi^{\left(\beta_{1} \ldots \beta_{n}\right)}\right|_{t=0} \\
&+\int_{0}^{t} G_{\beta_{1}}^{\alpha_{1}}\left(t, t^{\prime}\right) \ldots G_{\beta_{n}}^{\alpha_{n}}\left(t, t^{\prime}\right) f_{m}^{\left(\beta_{1}, \ldots \beta_{n}\right)}\left(t^{\prime}\right) \mathrm{d} t^{\prime} . \tag{6.3}
\end{align*}
$$

In principle, this can be applied repeatedly to increase the accuracy of the moments to whatever order is required.

## 7. The evolution of the centroid and of moments relative to it

The evolution of the centroid relative to some basal trajectory is a special case of (6.3) with $n=1$. Thus

$$
\begin{equation*}
\left\langle x^{\alpha}\right\rangle=\xi^{\alpha}+\int_{0}^{t} G_{\beta}^{\alpha}\left(t, t^{\prime}\right) f_{m}^{\beta}\left(t^{\prime}\right) \mathrm{d} t^{\prime}+\mathrm{O}(m+2) \tag{7.1}
\end{equation*}
$$

where $\xi^{\alpha}$ has been chosen such that $\xi^{\alpha}(0)=\left\langle x^{\alpha}\right\rangle_{t=0}$. This generalises an earlier result (Andrews 1981a, equation (4.2)) to arbitrary Hamiltonians and to arbitrary orders of accuracy.

The moments relative to the centroid can readily be found from those relative to the basal trajectory. Some low-order cases were considered earlier (Andrews 1983, §6). The general transformation to the moment ${\underset{\chi}{\chi}}^{\alpha_{1} \ldots \alpha_{n}}$ relative to the centroid can be written as

$$
\begin{gather*}
\underline{\chi}^{\alpha_{1} \ldots \alpha_{n}}=\chi^{\alpha_{1} \ldots \alpha_{n}}+\sum_{k=1}^{n-2}(-1)^{k} \sum_{i_{1}<\ldots<i_{k}} \chi^{\alpha_{i_{1}}} \ldots \chi^{\alpha_{i_{k}}} \chi^{\beta_{1} \ldots \beta_{n-k}} \\
+(-1)^{n-1}(n-1) \chi^{\alpha_{1}} \ldots \chi^{\alpha_{n}} \tag{7.2}
\end{gather*}
$$

where $\beta_{1} \ldots \beta_{n-k}$ denotes the set $\alpha_{1} \ldots \alpha_{n}$ with $\alpha_{i_{1}} \ldots \alpha_{i_{k}}$ removed. The inverse transformation is

$$
\begin{equation*}
\chi^{\alpha_{1} \ldots \alpha_{n}}=\underline{\chi}^{\alpha_{1} \ldots \alpha_{n}}+\sum_{k=1}^{n-2} \sum_{i_{1}<\ldots<i_{k}} \chi^{\alpha_{i_{1}}} \ldots \chi^{\alpha_{i_{k}}} \underline{\chi}^{\beta_{1} \ldots \beta_{n-k}}+\chi^{\alpha_{1}} \ldots \chi^{\alpha_{n}} . \tag{7.3}
\end{equation*}
$$

By definition, $\underline{\chi}^{\alpha}=0$.

## 8. Direct calculation of moments relative to the centroid

One normally seeks moments relative to the centroid and these, in general, will grow more slowly than those relative to a classical trajectory. One would therefore expect that an expansion in terms of the former moments would converge more rapidly and be more widely applicable. Unfortunately such a scheme is more complicated; it is necessary to increase the order of accuracy of the centroid and the other moments alternately and at each step to solve a new coupled set of differential equations for functions analogous to $u^{\alpha}{ }_{\beta}$.

Since $\xi^{\alpha}$ now represents the centroid as well as the reference trajectory, we will use $\xi_{m}^{\alpha}$ to denote an approximation accurate to order $m$; thus

$$
\begin{equation*}
\xi_{m}^{\alpha}=\xi^{\alpha}+\mathrm{O}(m+1) \tag{8.1}
\end{equation*}
$$

The evolution of $\xi$ is given from (5.2) as

$$
\begin{equation*}
\dot{\xi}^{\alpha}=\phi^{\alpha}+\sum_{k=2}^{\infty}(1 / k!) \phi_{\gamma_{1} \ldots \gamma_{k}}^{\alpha} \chi^{\gamma_{1} \ldots \gamma_{k}} . \tag{8.2}
\end{equation*}
$$

Since

$$
\phi^{\alpha}\left(\xi_{m}\right)=\phi^{\alpha}\left(\xi_{m-1}\right)+\left(\xi_{m}^{\beta}-\xi_{m-1}^{\beta}\right) \phi_{\beta}^{\alpha}\left(\xi_{m-1}\right)+\mathrm{O}(2 m)
$$

a suitable approximation of $\xi_{m}$ can be found from

$$
\begin{equation*}
\dot{\xi}_{m}^{\alpha}=\phi_{\beta}^{\alpha}\left(\xi_{m-1}\right) \xi_{m}^{\beta}+g_{m}^{\alpha} \tag{8.3}
\end{equation*}
$$

with the initial condition

$$
\begin{equation*}
\xi_{m}^{\alpha}(0)=\left.\left\langle x^{\alpha}\right\rangle\right|_{r=0} \tag{8.4}
\end{equation*}
$$

where
$\mathrm{g}^{\alpha}{ }_{m}:=\phi^{\alpha}\left(\xi_{m-1}\right)-\xi_{m-1}^{\beta} \phi^{\alpha}{ }_{\beta}\left(\xi_{m-1}\right)+\sum_{k=2}^{\infty}(1 / k!) \phi^{\alpha}{ }_{\gamma_{1} \ldots \gamma_{k}}\left(\xi_{m-1-a_{k}}\right) \chi_{m-1-\gamma_{k}}^{\gamma_{k} \ldots \gamma_{k}}$
and the $a_{2}, a_{3}, \ldots, a_{m}, c_{2}, c_{3}, \ldots, c_{m}$ are arbitrary integers subject to $a_{k}, c_{k} \leqslant k-1$.
For $m=0$, we take $\xi_{0}^{\alpha}$ to be the basal trajectory. Then $\xi_{1}^{\alpha}$ is also the basal trajectory, since (8.2) shows that $\langle x\rangle=\xi_{0}+\mathrm{O}(2)$.

The calculation scheme must be arranged so that $g_{m}^{\alpha}$ is known as a function of time and then (8.3) can be solved in the same way as was (6.1) via (6.3) using the solutions of $\dot{u}^{\alpha}{ }_{\beta}(t)=\phi^{\alpha}{ }_{\gamma}\left(\xi_{m-1}\right) u^{\gamma}{ }_{\beta}$ as before. Since the $\xi_{m}$ do not satisfy an equation of the form $\dot{\xi}^{\alpha}=\phi^{\alpha}$, these functions $u^{\alpha}{ }_{\beta}$ cannot be obtained by differentiation of trajectories.

Having found $\xi_{m}^{\alpha}$, the moments accurate to order $m+n$ can be found from

$$
\begin{equation*}
\dot{\chi}_{m}^{\alpha_{1} \ldots \alpha_{n}}=\sum_{i=1}^{n} \phi_{\gamma}^{\alpha_{1}}\left(\xi_{m}\right) \chi^{\alpha_{1} \ldots \alpha_{[1}, \gamma \alpha_{i+1} \ldots \alpha_{n}}+g_{m}^{\alpha_{1} \ldots \alpha_{n}} \tag{8.6}
\end{equation*}
$$

with

$$
\left.\chi_{m}^{\alpha_{1} \ldots \alpha_{n}}\right|_{t=0}=\left.\chi^{\alpha_{1} \ldots \alpha_{n}}\right|_{t=0}
$$

where

$$
\begin{align*}
& g_{m}^{\alpha_{1} \ldots \alpha_{n}}:=\sum_{i=1}^{n} \sum_{k=2}^{m+1} \frac{1}{k!} \phi_{\gamma_{1} \ldots \gamma_{k}}^{\alpha_{i}}\left(\xi_{m-1-a_{k}}\right) \\
& \times\left(\chi_{m-1-b_{k}}^{\alpha_{1} \ldots \alpha_{i-1}, \gamma_{1} \ldots \gamma_{k} \alpha_{i+1} \ldots \alpha_{n}}-\chi_{m-1-c_{k}}^{y_{1}, \gamma_{k}} \chi_{m-1-d_{k}}^{\alpha_{1}, \alpha_{i-1} \alpha_{i-1} \ldots \alpha_{n}}\right) \tag{8.7}
\end{align*}
$$

subject to $a_{k}, b_{k}, c_{k}, d_{k} \leqslant k-2$. Again the symmetrised approximate moments can be found as in (6.3), and the general moments from these.

Of course the $u^{\alpha}{ }_{\beta}$ and $G_{\beta}^{\alpha}$ must be recalculated at each order of accuracy and the work involved is therefore much greater than for the scheme based on moments relative to the basal trajectory.

## 9. Discussion

A striking outcome of the preceding development is the special role of the symmetrical moments. This is brought out strongly in the case of quadratic Hamiltonians. For these it follows from Ehrenfest's theorem that the centroid follows a classical trajectory. It is not difficult to show that all symmetrical moments have the same evolution equations as do classical moments under the corresponding classical Hamiltonian. If the quantum system and the classical cluster are taken to have the same symmetrised moments at some time, then these moments will be the same for all time. It should be noted, however, that some sets of values of the moments which are possible for a cluster are inaccessible to quantum systems because of the uncertainty relations (Andrews 1981a, §5). Of course quadratic Hamiltonians are well known to have special properties and there is already a considerable literature on the evolution of their moments (e.g. Hasse 1978, Remaud and Hernandez 1980).

For arbitrary quantum Hamiltonians, even the symmetrical moments do not have the same evolution as classical moments but the difference is of order $\hbar^{2}$ (where it is assumed that the Hamiltonian is Hermitian and independent of $\hbar$ ). Since all moments can be expressed in terms of the symmetrical ones, this can be encompassed by the more general semiclassical result
$\chi_{\text {quantum }}^{\alpha_{1} \ldots \alpha_{n}}=\chi_{\text {classical }}^{\alpha_{1} \ldots \alpha_{n}}+\frac{1}{2} i \hbar \sum_{p=q} \varepsilon^{\alpha_{p} \alpha_{4}} \chi_{\text {classical }}^{\alpha_{1} \cdot \alpha_{j}}{ }^{\alpha_{p+1}} \ldots \alpha_{q-1} \alpha_{q+1} \alpha_{n}+\mathrm{O}\left(\hbar^{2}\right)$,
where again it has been assumed that $\chi_{\text {quantum }}^{\left(\alpha_{1} \ldots \alpha_{n}\right)}=\chi_{\text {classical }}^{\alpha_{1}, \alpha_{y}}$ at $t=0$ and that the Hamiltonian is Hermitian and independent of $\hbar$. To prove (9.1), add (4.4) to the result of reversing the order of $\alpha_{1} \ldots \alpha_{n}$ and use $\chi^{\alpha_{1} \ldots \alpha_{n}}+\chi^{\alpha_{n} \cdots \alpha_{1}}=2 \chi^{\left.i \alpha_{1} \ldots \alpha_{n}\right)}+\mathrm{O}\left(\hbar^{2}\right)$, which follows from (4.3) of Hall (1985).

Equation (9.1) seems to imply that the classical limit associated with a wavepacket is not a trajectory but a cluster or classical distribution. How can one find such a classical distribution which has initially the same moments as the symmetrical moments of a given quantum system? The answer to this follows from the results that Weyl's rule applied to products of powers yields symmetrised products (Hall 1985). Thus a suitable classical distribution is given by the Wigner distribution.

Home and Sengupta (1983) take the interesting view that the appropriate classical limit is an ensemble of classical particles. They found, for three particular quadratic
potentials and for initially Gaussian wavepackets, that the time-evolution of Wigner distribution agrees with the Schrödinger evolution of the quantum wavepacket. They appear to conjecture that this wll be true generally but, in the light of the comments preceding equation (6.1), this cannot be so.

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