GRADIENT EXPANSIONS AND QUANTUM MECHANICAL EXTENSIONS OF THE

CLASSICAL PHASE SPACE

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INTRODUCTION

One common feature of most derivations of the gradient expansion for the kinetic energy density is the use of a mock phase space in intermediate steps. By mock phase space I mean a space parametrized by two coordinates p and r which in the classical limit reduce to the classical phase space. Of course a real phase space can not be defined quantum mechanically since p and r can not be specified simultaneously. Also there are many different mock phase spaces of which two in particular are frequently used. We will discuss these two in detail later. I will begin by giving a brief derivation of the Thomas-Fermi relation between the kinetic energy density and the spatial density to motivate the use of phase space and then indicate how this must be generalized. I then will discuss the various quantum mechanical generalizations of the phase space and show using the Wigner transform as an example one method of obtaining an $\hbar$ expansion. More details can be found in a review article by N.L. Balazs and myself.¹

MOCK PHASE SPACES

In the limit when $\hbar$ is small we can write the phase space density for fermions as

$$f_{c1}(p,r) = \theta\left(\lambda - \frac{p^2}{2m} - V(r)\right) \quad (1)$$

where $V(r)$ is a one-body potential. The density and kinetic energy density can be written as

$$\rho(r) = \int d^3p f_{c1}(p,r) \sim (\lambda - V(r))^{3/2} \quad (2)$$

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and

$$\tau(r) = \int d^3p \frac{p^2}{2m} f_{c1}(p,r) \sim (\lambda - V(r))^{5/2} \quad (3)$$

respectively. From this the well known Thomas-Fermi result $\tau(r) \sim \rho(r)^{5/3}$ follows immediately. To extend this procedure to obtain the gradient expansion it is necessary to perform the following steps: 1) Define $f(p,r)$ quantum mechanically; 2) Expand $f(p,r)$ in powers of $\hbar$; 3) Compute $\rho(\lambda - V(r))$ and $\tau(\lambda - V(r))$ term by term in $\hbar$; and 4) Express τ as a functional of ρ by eliminating V .

Let me now discuss the first step, i.e. defining $f(p,r)$. Quantum mechanically a probability is found by taking a trace. Thus the probability for finding a particle at a point r is

$$\text{Pr}(r) = \text{Tr } \delta(r - \hat{r}) \hat{\rho} = \langle r | \hat{\rho} | r \rangle \quad (4)$$

where $\hat{\rho}$ is one body density matrix and the $\hat{}$ denotes operators. Similarly for the momentum distribution

$$\text{Pr}(p) = \text{Tr } \delta(p - \hat{p}) \hat{\rho} = \langle p | \hat{\rho} | p \rangle \quad (5)$$

The most naive method of attempting to define a joint probability is then

$$f_g(p,r) = \text{Tr } \delta(p - \hat{p}) \delta(r - \hat{r}) \hat{\rho} = \langle r | \hat{\rho} | p \rangle \langle p | r \rangle \quad (6)$$

and most other putative quantum mechanical phase space densities are simple generalizations of this obtained through different orderings of the $\hat{p}$ and $\hat{r}$ operators. When $\hat{\rho} = \theta(\lambda - \hat{H})$ the $f_g(p,r)$ defined by Eq. (6) is just the function used by E.K.U. Gross² in his lecture on the Kirzhnits method.³ He wrote the density as

$$\rho = \int d^3p \langle r | \theta(\lambda - \hat{H}) | p \rangle \langle p | r \rangle \quad (7)$$

and did an $\hbar$ expansion on the integrand. In the Wigner-Kirkwood expansion⁴ one works with the Laplace transform of $f_g(p,r)$ (see Ref. 1 for a discussion of the Wigner-Kirkwood expansion from this point of view). Note that the $f_g(p,r)$ defined by Eq. (6) is not the Wigner distribution function.

The delta functions in Eq. (6) can be written through the Fourier transform. Thus we have

$$\begin{aligned} \hat{\Delta}_g(p,r) &= \delta(p - \hat{p}) \delta(r - \hat{r}) \\ &= \frac{1}{(2\pi)^6} \int d^3u d^3v \exp(iu \cdot (p - \hat{p}) + iv \cdot (r - \hat{r})) \\ &= \frac{1}{(2\pi)^6} \int d^3u d^3v \exp(iu \cdot (p - \hat{p}) + iv \cdot (r - \hat{r})) \exp\left(\frac{i\hbar u \cdot v}{2}\right) \end{aligned} \quad (8)$$

In the last line the phase $i\hbar\mathbf{u}\cdot\mathbf{v}/2$ has come from combining the two exponentials. We can define a new $\hat{\Delta}$ by dropping the phase. Thus we have

$$\hat{\Delta}_w = \frac{1}{(2\pi)^6} \int d^3u d^3v \exp(i\mathbf{u}\cdot(\mathbf{p}-\hat{\mathbf{p}}) + i\mathbf{v}\cdot(\mathbf{r}-\hat{\mathbf{r}})) . \quad (9)$$

This new $\hat{\Delta}$ differs from $\hat{\Delta}_g$ just in the ordering of the $\hat{\mathbf{p}}$ and $\hat{\mathbf{r}}$ operators. It is Hermitian and symmetric in $\hat{\mathbf{p}}$ and $\hat{\mathbf{r}}$. We can now define a new distribution function

$$f_w(\mathbf{p}, \mathbf{r}) = \text{Tr} \hat{\Delta}_w(\mathbf{p}, \mathbf{r}) \hat{\rho} . \quad (10)$$

This is the Wigner distribution function. Given either $f_w(\mathbf{p}, \mathbf{r})$ or $f_g(\mathbf{p}, \mathbf{r})$ the full off diagonal density matrix may be easily reconstructed. While $f_g(\mathbf{p}, \mathbf{r})$ is in general complex $f_w(\mathbf{p}, \mathbf{r})$ is real although it can be negative. Thus neither f_g or f_w is a true probability. In many cases $f_g(\mathbf{p}, \mathbf{r})$ can be more easily calculated than $f_w(\mathbf{p}, \mathbf{r})$. For example the lack of symmetry between $\mathbf{p}$ and $\mathbf{r}$ in $f_g(\mathbf{p}, \mathbf{r})$ is exploited in deriving the Wigner-Kirkwood expansion.^{4,1}

The two f 's are related by

$$f_w(\mathbf{p}, \mathbf{r}) = \exp \frac{i\hbar \nabla \cdot \mathbf{V}}{2} f_g(\mathbf{p}, \mathbf{r}) . \quad (11)$$

From this equation it should not be concluded that $f_w(\mathbf{p}, \mathbf{r})$ and $f_g(\mathbf{p}, \mathbf{r})$ are equal when $\hbar \rightarrow 0$ since both may be rapidly oscillating and the gradients in effect go like $1/\hbar$. However, if there is averaging the two will become the same.

For any operator $\hat{O}$ it is possible to define a function

$$O_g(\mathbf{p}, \mathbf{r}) = \text{Tr} \hat{\Delta}_g(\mathbf{p}, \mathbf{r}) \hat{O} \quad (12)$$

and thus with each operator associate a function of $\mathbf{p}$ and $\mathbf{r}$. (One can proceed similarly with Δ_w .) The point of this is that all of quantum mechanics can be recast in terms of these associated functions rather than the original operators.¹

I have by no means exhausted the possible choices for $\hat{\Delta}$. For almost every ordering it is possible to generate a new $\hat{\Delta}$. Thus there is a tremendous freedom which can be exploited in the solution of individual problems.

THE $\hbar$ EXPANSION

In this section I will present a method of obtaining the $\hbar$ expansion first given by Voros.⁵ In this method the density matrix $\hat{\rho} = \mathcal{Q}(\lambda - \hat{H})$ is formally expanded about a c -number. Thus we have

$$\begin{aligned} \hat{\rho} &= \mathcal{Q}(E - \hat{H}) = \mathcal{Q}(E - \hat{\mathcal{N}} + (\hat{\mathcal{N}} - \hat{H})) \\ &= \mathcal{Q}(E - \hat{\mathcal{N}}) + (\hat{\mathcal{N}} - \hat{H}) \frac{\partial}{\partial E} \mathcal{Q}(E - \hat{\mathcal{N}}) \\ &\quad + \frac{1}{2} (\hat{\mathcal{N}} - \hat{H})^2 \frac{\partial^2}{\partial E^2} \mathcal{Q}(E - \hat{\mathcal{N}}) + \dots \end{aligned} \quad (13)$$

The Wigner transform is now taken term by term. Thus

$$\begin{aligned} f_w(\mathbf{p}, \mathbf{r}) &= \text{Tr} \hat{\Delta}_w \mathcal{Q}(E - \hat{H}) \\ &= \mathcal{Q}(E - \mathcal{N}) \text{Tr} \hat{\Delta} + \delta(E - \mathcal{N}) \text{Tr} \{ \hat{\Delta} (\hat{\mathcal{N}} - \hat{H}) \} \\ &\quad + \frac{1}{2} \delta'(E - \mathcal{N}) \text{Tr} \{ \hat{\Delta} (\hat{\mathcal{N}} - \hat{H})^2 \} + \dots \end{aligned} \quad (14)$$

I could equally well have used $\hat{\Delta}_g$ and $f_g(\mathbf{p}, \mathbf{r})$ rather than $\hat{\Delta}_w$ and $f_w(\mathbf{p}, \mathbf{r})$. The latter was chosen simply for the sake of definiteness. To evaluate Eq. (14) it is only necessary to calculate $\text{Tr} \hat{\Delta}(\hat{H})^N$ for various values of N . The $\hbar$ corrections arise because

$$(\text{Tr} \hat{\Delta}(\hat{H})^N \neq \text{Tr} \hat{\Delta}(\hat{H})^N . \quad (15)$$

Now we must decide how to choose $\mathcal{N}$. One possibility is $\mathcal{N} = \text{Tr} \hat{\Delta} \hat{H}$. Thus a different $\mathcal{N}$ is chosen for each point in the $\mathbf{p}, \mathbf{r}$ plane i.e. $\mathcal{N}$ is a function of $\mathbf{p}$ and $\mathbf{r}$. For the normal Hamiltonian $\hat{H} = \hat{\mathbf{p}}^2/2m + V(\hat{\mathbf{r}})$, $\mathcal{N}$ is independent of $\hbar$ and the $\hbar$ expansion of $f_w(\mathbf{p}, \mathbf{r})$ is obtained by rearranging terms in Eq. (14). Thus we have

$$\begin{aligned} f_w(\mathbf{p}, \mathbf{r}) &= \mathcal{Q}(E - \mathcal{N}(\mathbf{p}, \mathbf{r})) + \hbar^2 \left\{ -\delta'(E - \mathcal{N}) \frac{\nabla^2 V}{8m} \right. \\ &\quad \left. + \delta''(E - \mathcal{N}) \left[\frac{(\nabla V)^2}{24m} + \frac{(\mathbf{p} \cdot \nabla)^2 V}{24m^2} \right] \right\} \\ &\quad + \mathcal{O}(\hbar^4) . \end{aligned} \quad (16)$$

Note that in Eq. (16) there is no term proportional to $\hbar$ and $f_w(\mathbf{p}, \mathbf{r})$ is real. If we had used $f_g(\mathbf{p}, \mathbf{r})$ instead there would have been an imaginary term proportional to $\hbar$. The above procedure is easily extended to more complex Hamiltonians.⁶

The rest of the procedure in obtaining the gradient expansion for the kinetic energy is rather tedious and not particularly enlightening so I will not go through it here. It is discussed in Refs. 1, 2, 3 and 6.

ACKNOWLEDGEMENTS

I would like to thank the organizers of this conference for asking me to give this contribution and the Natural Sciences and Engineering Research Council of Canada for financial support.

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