The Thermal Content of Quantum States

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It is shown that the exact structure of Schrödinger Quantum Mechanics is a consequence of the assumption that there exist two subquantum fluids in local thermal equilibrium.

Introduction

There is a long history of attempts to establish that Schrödinger quantum mechanics is explicable in terms of the familiar classical concepts and formalisms such as particle trajectories, Probability flow, Phase space densities, Fluid dynamics, Stochastic theory, etc., (see Ref. [1-10]). There are varying degrees of success, failure and controversy surrounding these attempts. Often the ideas behind such theories are highly plausible but either the mathematical formulation falls short of being convincing or some of the analogies revealed are still difficult to appreciate in ordinary classical terms. This last mentioned type of difficulty occurs in the line of work which appears to have originated from a paper by MADELUNG [1] on the fluid analogy for quantum mechanics. The main trouble here lies in the form and interpretation of the "quantum potential" [Ref. [2], Eq. (2a)]

$$\frac{\hbar^2}{4\,m}\left[\frac{1}{2}\left(\frac{\nabla \varrho}{\varrho}\right)^2 - \frac{\nabla^2 \varrho}{\varrho}\right] \tag{1}$$

for which it has seemed to be impossible to find any convincing classical image or explanation. Expression (1) can be regarded as the manifestation of a pressure [8] and with this interpretation the fluid analogy is complete, but why the pressure in the quantum probability fluid should assume this odd form involving derivatives of the density has been something of a mystery. In this paper we shall give a convincing explanation for the inevitability of the form (1) in terms of a very plausible assumption about the interaction of the "fluids" involved. The existence of two fluids and not just one is the clue that has been missing and the plausible assumption is that the two fluids are in local thermal equilibrium.

The Basic Structure

The physical picture we have in mind can take a number of possible forms. In particular, we can think of the solvent, solute situation, of two mutually miscible fluids or, indeed, the "Brownian" motions of particles suspended in a fluid. The latter image has been given a mathematical form by NELSON [6] but here the mathematical form does not seem to coincide at all closely with quantum mechanics [10]. The danger in giving, a priori, too precise a physical form to our basic structure is that we are then tempted to apply equations appropriate to that particular physical picture, only to find that our densities are over defined or inconsistent with the superstructure (quantum mechanics) which we wish to generate. The minimum necessary assumption which will meet our requirements is that we are dealing with a two component fluid like system. The exact physical dress to be worn by the two interacting fluids is a matter for further study in terms of their defined and necessary characteristics. We shall here just use this minimum concept that two fluids are interacting to form our substructure, and for convenience of visualisation we shall use the terminology of the solvent solute situation.

The Joint Phase Space Distribution

Apart from the idea of two interacting fluids our mathematical equipment will include a general, but at first unknown, time dependent phase-space distribution, $g(x, t, p', p)$. This distribution will be regarded as, in some sense, representing the local state of the two fluid system at position x and at time t. The momentum variable, p', will refer to the back-

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ground fluid (solvent) motion and the momentum variable, p, will refer to the object or particle (solute) in its motion through the background fluid. The idea here is to decompose the usual conceptual quantum particle into two components. The two structural parts being the "particle" (solute) and the "vacuum" (solvent). The existence of a contribution to a quantum state at the position x in configuration space can be regarded as having the consequence of causing the "vacuum" (solvent) to react and so locally either to take up or supply some energy to the "particle" according to its state of stress caused by the "particle" (solute) distribution. Thus locally the natural zero for the "particle" energy density is the local energy density for the stressed vacuum. This particular complication is not noticed in conventional quantum theory because the concept of local energy density is not important in most applications. There only the global [11] energy is usually considered.

We shall at this stage make no assumptions about the actual form that $g(x, t, p', p)$ should take. We cannot assume that g is a Maxwell distribution [6, 8] or any such form peculiar to the Fokker-Planck equation. It is true that a generalization of quantum theory can be put into the form of a Fokker-Planck equation for density [11] but this theory involves a time element, τ, which arises from approximating and it was shown in Ref. [11] that the Fokker-Planck equation is a consequence of the approximation and so is 'outside' conventional quantum theory which arises when $\tau \to 0$. Here we wish to work in such a way that our formalism at least contains a part which is exactly equivalent to conventional quantum theory.

Thermal Equilibrium

The final and all important key assumption necessary to our argument is that the two fluids are in thermal equilibrium at all points of configuration space. Further, this assumption is not only confined to steady states but is taken to hold quite generally over the whole range of quantum possibilities. Thus in general if the heat density of the "particle" at position x and time t is denoted by μ (solute $| x, t$),

and the heat density of the stressed vacuum at position x and time t is denoted by μ (solvent $| x, t$); then our key assumption that there is thermal equilibrium has the simple form

$$\mu(\text{solute} \,|\, x, t) + \mu(\text{solvent} \,|\, x, t) = 0. \qquad (2)$$

Using $g(x, t \,|\, p', p)$ we can now write down the various functions needed to give detailed expression to Eq. (2). The usual definitions from the statistical theory of fluids [12, 13] are used.

We shall require the local average momenta for solute and solvent which are

$$\bar{p}(x, t) = \iint p \, g(x, t \,|\, p', p) \, \mathrm{d}p' \, \mathrm{d}p \qquad (3)$$

and

$$\bar{p}'(x, t) = \iint p' \, g(x, t \,|\, p', p) \, \mathrm{d}p' \, \mathrm{d}p \qquad (4)$$

respectively.

The two local thermal energy densities are then given by

$$\mu(\text{solute} \,|\, x, t) = \iint \frac{(p - \bar{p})^2}{2\,m} \, g(x, t \,|\, p', p) \, \mathrm{d}p' \, \mathrm{d}p \qquad (5)$$

and

$$\mu(\text{solvent} \,|\, x, t) = \iint \frac{(p' - \bar{p}')^2}{2\,m} \, g(x, t \,|\, p', p) \, \mathrm{d}p' \, \mathrm{d}p . \qquad (6)$$

When the solute is also subject to the influence of an external potential $W(x, t)$, its total energy density will be

$$E(\text{solute}) = \iint \frac{p^2}{2\,m} \, g(x, t \,|\, p', p) \, \mathrm{d}p' \, \mathrm{d}p + W. \qquad (7)$$

The energy density of the solvent will be

$$E(\text{solvent}) = \iint \frac{p'^2}{2\,m} \, g(x, t \,|\, p', p) \, \mathrm{d}p' \, \mathrm{d}p . \qquad (8)$$

As remarked earlier, the natural local zero of energy for the "particle" will be that of the stressed vacuum. Thus we shall define the local quantum energy density, E_Q, by

$$E_Q = E(\text{solute}) - E(\text{solvent}) \qquad (9)$$

and then by (5), (6), (7) and (8), definition (9) gives

$$E_Q = \frac{\bar{p}^2}{2\,m} - \frac{\bar{p}'^2}{2\,m} + \mu(\text{solute}) - \mu(\text{solvent}) \qquad (10)$$

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[12] S. A. RICE and P. GRAY, The Statistical Mechanics of Simple Liquids, Interscience 1965.
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$$= \frac{\bar{p}^2}{2\,m} - \frac{\bar{p}'^2}{2\,m} + 2\,\mu\,(\text{solute}). \qquad (11)$$

The last form arising from the condition for local thermal equilibrium (2).

The form (11) is already very near the mark as can be seen by taking

$$E_Q = \text{Re}\; i\,\hbar\, \frac{\partial \log \psi}{\partial t} \quad \text{and} \quad \bar{p} + i\,\bar{p}' = -\,i\,\hbar\, \frac{\partial \log \psi}{\partial q}$$

on the assumption that ψ is a solution to the Schrödinger equation [see Ref. [11], Eq. (46)], but we can do better than this. We have not yet made any explicit use of the distribution $g(x,t\,|\,p',p)$ and this we shall do next.

Identifying the variables p and p'

If we express (2) in terms of (5) and (6) we get the relation

$$\iint \left\{ \frac{(p-\bar{p})^2}{2\,m} + \frac{(p'-\bar{p}')^2}{2\,m} \right\} g(x,t\,|\,p',p)\;\mathrm{d}p'\,\mathrm{d}p = 0. \qquad (12)$$

If (12) is to hold in other than the trivial sense ($g \equiv 0$) then g cannot simply be a pure probability distribution. This is an important clue to the form that g must take. It must, clearly, be negative [15] in some regions of phase space.

This suggests trying for g a function related to WIGNER's phase space distribution [14] $F(p,q)$ which is well-known to have negative regions. Further, there is the advantage that the $F(p,q)$ are unambiguously related to conventional quantum states [11,16]. However, we need here a dependence on two momentum variables, p and p', and so the plain $F(p,q)$ will do not. A little thought leads one to try introducing p' analogously to the way p occurs in $F(p,q)$ and thus one arrives at the form

$$g(x,t\,|\,p',p) \qquad (13)$$
$$= \frac{\varrho^{-1}}{(2\,\pi)^2} \iint \Gamma(x,t,\tau_1,\tau_2)\, e^{-i(\tau_1 p + \tau_2 p')}\,\mathrm{d}\tau_1\,\mathrm{d}\tau_2,$$

where

$$\Gamma(x,t,\tau_1,\tau_2) = \psi^*\!\left(x - \frac{\hbar\,\tau}{2}\,,\,t\right) \psi\!\left(x + \frac{\hbar\,\tau^*}{2}\,,\,t\right), \qquad (14)$$

$$\tau = \tau_1 + i\,\tau_2, \qquad (15)$$

and
$$\varrho = \psi^*(x,t)\,\psi(x,t). \qquad (16)$$

The function $g(x,t\,|\,p',p)$ has the property

$$\int\limits_{-\infty}^{+\infty} g(x,t\,|\,p',p)\;\mathrm{d}p' = \varrho^{-1}\,F(p,x). \qquad (17)$$

The form (13) turns out to be completely correct with (2) holding rigorously. Boundary terms at $\tau = \pm\,\infty$ are eliminated by restricting to those Γ for which

$$\lim_{\tau \to \pm\infty} \Gamma = 0 \quad \text{and} \quad \lim_{\tau \to \pm\infty} \frac{\partial \Gamma}{\partial \tau} = 0. \qquad (18)$$

Further, on using (13) to calculate $\bar{p}$, $\bar{p}'$ and μ in terms of $\psi(x,t)$, one finds that

$$p = -\,\text{Re}\!\left(i\,\hbar\, \frac{\partial \log \psi}{\partial x}\right), \qquad (19)$$

$$\bar{p}' = -\,\text{Im}\!\left(i\,\hbar\, \frac{\partial \log \psi}{\partial x}\right) = -\,\frac{\hbar}{2}\, \frac{\partial \log \varrho}{\partial x} \qquad (20)$$

and

$$\mu\,(\text{solute}) = -\,\frac{\hbar^2}{8\,m}\, \frac{\partial^2 \log \varrho}{\partial x^2}. \qquad (21)$$

These can now be substituted into (11) to give

$$E_Q = \frac{\bar{p}^2}{2\,m} + \frac{\hbar^2}{4\,m}\left\{ \frac{1}{2\,\varrho^2}\left(\frac{\partial\varrho}{\partial x}\right)^2 - \frac{1}{\varrho}\, \frac{\partial^2\varrho}{\partial x^2} \right\} \qquad (22)$$

$$\equiv \frac{\bar{p}^2}{2\,m} - \int \frac{(\text{pressure})}{\varrho}\,\mathrm{d}x. \qquad (23)$$

Expression (22) is exactly the quantum formula for local energy density in the Schrödinger form [11]. The second form (23) identifies the pressure [8]. Thus we now see clearly how this pressure term arises. It is, in fact, a consequence of the thermal interaction of the particle with its local stressed vacuum.

Conclusions

This work would seem to prove conclusively that the fluid dynamical aspect of Schrödinger quantum mechanics should be taken seriously and the implications of the thermal equilibrium which has been shown to be fundamental should be fully explored.

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