A remark on the connection between stochastic
mechanics and the heat equation

by

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ABSTRACT

We prove that the solution of Nelson's stochastic mechanics equation associated with any stationary solution ψ of the Schrödinger equation is the homogeneous Markoff process of the heat equation with Dirichlet boundary condition on the hypersurface $\psi = 0$.

1. Introduction.

In [1] Nelson introduced the concept of stochastic mechanics and discussed its relations with quantum mechanics. This opens the possibility of discussing quantum mechanical questions in terms of Markov processes as well as studying Markov processes by the techniques used in quantum mechanics. We shall sketch Nelsons argument for the case of a system with n degrees of freedom and a conservative force field $-\nabla V$. For simplicity we set all the masses equal to one.

Starting with the Schrödinger equation

$$i \frac{\partial}{\partial t} \psi(x,t) = -\frac{1}{2} \Delta \psi(x,t) + V(x) \psi(x,t) , \quad (1)$$

we write the solution in the form

$$\psi(x,t) = \rho^{\frac{1}{2}}(x,t) e^{iS(x,t)} \quad (2)$$

where $\rho = |\psi|^2$. Set $v(x,t) = \nabla S(x,t)$, where ∇ is the gradient with respect to x . Then a Markov process $\xi(t)$ in R^n is completely described by taking $\rho(x,t)$ to be the distribution of $\xi(t)$ and $v(x,t)$ its current velocity, i.e.

$$v(\xi(t),t) = \frac{1}{2}(D^+ + D^-) \xi(t) , \quad (3)$$

where D^+ and D^- are the mean forward and mean backwards derivatives:

$$D^{\pm} F(\xi(t),t) = \lim_{\epsilon \rightarrow 0^{\pm}} \epsilon^{-1} E_t[F(\xi(t+\epsilon),t+\epsilon) - F(\xi(t),t)] ,$$

where E_t is the conditional expectation with respect to $\xi(t)$.

If we define the displacement (drift) $\alpha(x,t)$ by

$$\alpha(x,t) = v(x,t) + \frac{1}{2} \nabla \ln \rho(x,t) \quad (4)$$

then it follows from the theory of stochastic differential equations that $\xi(t)$ satisfies the stochastic differential equation

$$d\xi(t) = \alpha(\xi(t), t)dt + dw(t) , \quad (5)$$

where $w(t)$ is the standard Brownian motion in R^n given by

$$E(dw_i(t)) = 0 , \quad E(dw_i(t) \cdot dw_j(t)) = \delta_{ij}dt .$$

It follows now from (1) that $\xi(t)$ satisfies the Newton equation in the form that the mean acceleration is equal to the force $-\nabla V$ i.e.

$$\frac{1}{2}(D^+D^- + D^-D^+) \xi(t) = -\nabla V(\xi(t)) . \quad (6)$$

On the other hand if we assume that we have a Markov process $\xi(t)$ which satisfies (5) and (6) for some function α of $\xi(t)$ and t , then we may define the function $\rho(x, t)$ as the distribution function for $\xi(t)$. It follows from (5) and (6) that the displacement $\alpha(x, t)$ is a gradient, so, if we now define $v(x, t)$ by (4), v is also a gradient. This gives us a real function $S(x, t)$ by $v = \nabla S$, where S is determined up to a constant. Defining now $\psi(x, t)$ by (2) Nelson proved that, under regularity conditions on the displacement $\alpha(x, t)$, $\psi(x, t)$ satisfies the Schrödinger equation (1). In the next section we shall see that in the case where $\alpha(x, t)$ is not regular enough then (5) and (6) have more solutions than those coming from (1). This was already noted by Nelson in [1].

Guerra and Ruggiero [2] have recently discussed the extension of Nelson's work to the case of the boson field. They make the very interesting observation that the corresponding Euclidian Markov field coincides with the lowest energy generalized stochastic process associated with classical field theory

through the procedure of Nelson's stochastic mechanics. So that in this sense the underlying four dimensional manifold on which the Markov field is defined can be considered as the physical space time. This has lead us to the considerations in the next section, where we shall discuss the relation between Nelson's stochastic mechanics and the heat equation for a system with n degrees of freedom.

2. Relations between stochastic mechanics and the heat equation.

The connection between the Schrödinger equation (1) and the corresponding heat equation

$$-\frac{\partial}{\partial t} \psi(x, t) = -\frac{1}{2} \Delta \psi(x, t) + V(x) \psi(x, t) \quad (7)$$

in the sense that the solution of (7) is analytic in $\operatorname{Re} t > 0$ and continuous for $\operatorname{Re} t \geq 0$ and their values on the imaginary axis are solutions of (1) has long been known and utilized, and it is this relation that forms the basis for Euclidian field theory. In this correspondence the parameter t in (7) has the interpretation of an imaginary time. However, by the observation made by Guerra and Ruggiero in [2] we are lead to the interpretation of the parameter t in (7) as the real physical time for the stationary process in stochastic mechanics corresponding to the groundstate for the Schrödinger equation (1). Hence by Nelson's equivalence between stochastic mechanics and quantum mechanics we are lead to the interpretation of the parameter t in (7) as the real physical time of quantum mechanics, at least for the ground state. We shall see below that such an interpretation also holds, with some modifications, for any stationary solution of (1).

Let us now assume that the potential $V(x)$ is such that (1) admits a stationary solution, i.e. a solution of the form $\psi(x, t) = e^{-i\lambda t} \varphi(x)$ with $\varphi(x) \in L_2(\mathbb{R}^n)$. So that

$$(-\frac{1}{2} \Delta + V - \lambda) \varphi = 0. \quad (8)$$

Since this is a real equation $\varphi(x)$ can always be chosen as a real function. In this case we have in the notations of the

previous section that $\rho = \varphi^2(x)$ and $S(x,t) = -\lambda t$. We remark that we have permitted the square root in (2) to be the positive or the negative square root, depending on whether $\varphi(x)$ is positive or negative i.e. $\rho^{\frac{1}{2}}(x) = \varphi(x)$. This is necessary in order to make $S(x,t)$ a continuous function of x . We now get that $v(x,t) = \nabla S = 0$. Hence the current velocity (3) for the Markov process $\xi(t)$ is zero. The corresponding displacement (drift) is therefore given by $\alpha(x,t) = \frac{1}{2} \nabla \ln \rho$. Let us assume that $V(x)$ is a smooth function so that by (8) $\varphi(x)$ is also a smooth function. In this case $\alpha(x,t)$ is a smooth function outside the set $\varphi(x) = 0$, where $\alpha(x,t)$ is given by

$$\alpha(x) = \frac{1}{\varphi(x)} \nabla \varphi(x). \quad (9)$$

Hence for a stationary solution of the Schrödinger equation, the current velocity satisfies $v(x,t) = 0$ and the displacement $\alpha(x)$ is equal to the osmotic velocity $\frac{1}{2} \nabla \ln \rho$, which is time independent and given in terms of the eigenfunction $\varphi(x)$ by (9). If $\varphi(x) > 0$ for all x then $\alpha(x)$ will satisfy regularity conditions sufficient to secure that the stochastic differential equation

$$d\xi(t) = \alpha(\xi(t))dt + dw(t) \quad (10)$$

has a solution and this solution is unique. See Ch. I § 3 of ref [3] and ref. [1]. So in this case we have a unique Markoff process $\xi(t)$ which is homogeneous in time with $\rho(x)$ as the distribution for $\xi(t)$ or, if we want, $\rho(x)dx$ as the invariant measure for the homogeneous process $\xi(t)$. The situation when $\varphi(x)$ has zeros is more complex since this leads, by (9), to singularities for the displacement $\alpha(x)$, and hence the above mentioned existence and uniqueness theorem does not apply.

We shall however show that even in this case there exist solutions of (10). The solution we construct is homogeneous with invariant distribution $\rho(x)$, which is related to $\alpha(x)$ by $\alpha(x) = \frac{1}{2} \nabla \ln \rho(x)$.

In fact let us look for solutions of

$$d\xi(t) = d(\xi(t))dt + dw(t) \quad (11)$$

where $\xi(t)$ is required to be a homogeneous Markov process with given invariant distribution $\rho(x)$ related to the displacement $\alpha(x)$ by

$$\alpha(x) = \frac{1}{2} \nabla \ln \rho(x) . \quad (12)$$

Since (12) implies that the displacement $\alpha(x)$ is equal to the osmotic velocity, we have that the current velocity $v(\xi(t), t) = \frac{1}{2}(D^+ + D^-) \xi(t)$ must be equal to zero because the displacement is $\alpha(\xi(t), t) = D^+ \xi(t)$ and the osmotic velocity is $\frac{1}{2} \nabla \ln \rho(x, t) = \frac{1}{2}(D^+ - D^-) \xi(t)$. Let $\xi_*(t)$ be the time reversed process. We then have that $D^- \xi_*(t) = -D^+ \xi(t)$ and by the fact that the current velocity of $\xi(t)$ is zero, we get

$$D^+ \xi_*(t) = D^+ \xi(t) , \quad (13)$$

which then gives that also the reversed process satisfies (11). It is therefore natural to seek solutions of (11) which satisfy the condition that $\xi_* = \xi$.

Since $\xi(t)$ has an invariant distribution $\rho(x)$ we may define a semigroup P_t in $L_2(\rho dx)$ by $(P_t f)(x) = E_0[f(\xi(t))]$ for any $f \in L_2(\rho dx)$, where E_0 is the conditional expectation with respect to $\xi(0)$. The condition $\xi_* = \xi$ implies that $P_t^* = P_t$, where P_t^* is the adjoint semigroup. It follows from the proof of theorem 3 ch. 2 § 9 of ref [3] that if $\xi(t)$ is a

solution of (11) and f is a smooth function which is zero in a neighborhood of the singularities of $\alpha(x)$, then the strong limit of $-\frac{1}{t} (P_t f - f)$ exists as $t \rightarrow 0$ and is given by

$$Af = -\frac{1}{2\rho} \nabla \cdot (\rho \nabla f) . \quad (14)$$

Hence we get that the infinitesimal generator A of P_t is a closed extension of the operator $-\frac{1}{2\rho} \nabla \cdot \rho \nabla$ defined on smooth functions which are zero near the zeros of ρ . The condition $\xi_* = \xi$ is equivalent to the condition $A = A^*$. Hence we know that if there is a solution of (11) with invariant distribution ρ and satisfying the condition $\xi = \xi_*$, then the semigroup P_t generated by the process is of the form $P_t = e^{-tA}$, where A is a self adjoint extension of $-\frac{1}{2\rho} \nabla \cdot \rho \nabla$ defined on smooth functions which are zero near the zeros of ρ . There is an obvious restriction for A , namely that we should have $\|P_t\| \leq 1$, E_0 being a conditional expectation, so that $A \geq 0$.

We may now identify $L_2(\rho dx)$ with $L_2(R^n)$ by the identification $f \leftrightarrow \varphi f$ since $\varphi^2 = \rho$. Then the operator $-\frac{1}{2\rho} \nabla \cdot \rho \nabla$ is identified with

$$-\frac{1}{2} \Delta + (V - \lambda) \quad (15)$$

since φ satisfies the equation $-\frac{1}{2} \Delta \varphi + (V - \lambda)\varphi = 0$. Hence in the $L_2(R^n)$ representation, $P_t = e^{-tA}$ where A is a positive selfadjoint extension of (15) defined on smooth functions which are zero near the zeros of $\varphi(x)$.

In the case λ is the lowest eigenvalue λ_0 we know that $\varphi(x)$ is always different from zero. Hence (15) is essentially self adjoint and for this special case we have then simply that $f(t, x) = (P_t f_0)(x)$ is the solution of the heat equation

$$-\frac{\partial}{\partial t} f = (-\frac{1}{2}\Delta + (V - \lambda_0))f, \quad (16)$$

with initial condition $f(0, x) = f_0(x)$. Hence in this case, which is also the case in which we have existence and uniqueness of (11), we get that the Markov process $\xi(t)$ of the stochastic mechanics is identical with the heat equation process described by (16).

In the case where λ is not the lowest eigenvalue we have that $\varphi(x)$ has zeros. In this case we take A to be the Friedrichs extension i.e. the minimal extension that conserves positivity of $-\frac{1}{2}\Delta + (V - \lambda)$ defined on smooth functions which are zero near the zeros of $\varphi(x)$. This is a self adjoint operator $A_\varphi \geq 0$, and it is well known that it is $-\frac{1}{2}\Delta_\varphi + (V - \lambda)$, where Δ_φ is the Laplacian with Dirichlet boundary conditions on the hypersurface $\varphi(x) = 0$. It follows then immediately that $\varphi(x)$ is in the domain of A_φ and that $A_\varphi \varphi(x) = 0$ so that $\rho(x)$ is an invariant measure for the process $\xi(t)$ generated by the probability semigroup $P_t^\varphi = e^{-tA_\varphi}$. Since the eigenfunction belonging to the lowest eigenvalue λ_0 for the eigenvalue problem (8) can be taken to be positive everywhere, we have that an eigenfunction φ belonging to any eigenvalue $\lambda > \lambda_0$ must take both positive and negative values. Hence the hypersurface $\varphi(x) = 0$ divides the space R^n into at least two disjoint domains. Let Λ_α , $\alpha = 1, \dots, e$ be the domains into which R^n is divided by the hypersurface $\varphi(x) = 0$. Since then Δ_φ is the direct sum of Δ_{Λ_α} operating in $L_2(\Lambda_\alpha)$, where Δ_{Λ_α} is the Laplacian with Dirichlet boundary conditions on the boundary of the domain Λ_α , we get that the process $\xi(t)$ given by P_t^φ does not have a unique invariant measure. We have namely that φ decomposes in a direct sum $\varphi = \sum_\alpha \varphi_\alpha$ with $\varphi_\alpha = \chi_{\Lambda_\alpha}$ such that

$P_t^\varphi \varphi_\alpha = \varphi_\alpha$. That is to say that all the distributions $\rho_\alpha = \varphi_\alpha^2$ are invariant distributions for the process. In fact we see that the process $\xi(t)$ given by P_t^φ never crosses the hyperplane $\varphi(x) = 0$, and if we start it in any of the connected domains Λ_α it will always remain there. However, if we restrict it to any of the domains Λ_α it has a unique invariant measure ρ_α . If we define $f(x, t) = (P_t^\varphi f_0)(x)$ we have

$$\frac{\partial}{\partial t} f = \left(-\frac{1}{2} \Delta_\varphi + (V - \lambda)\right) f. \quad (17)$$

So also in the case where φ is an eigenfunction not belonging to the lowest eigenvalue λ_0 we get that the Markoff process $\xi_\varphi(t)$ in the stochastic mechanics is identical with a heat equation process, namely the one described by (17). We summarize the above results in the following theorem.

Theorem 1. Let $\psi(x, t) = e^{-it\lambda} \varphi(x)$ be a stationary solution of the Schrödinger equation (1), with a smooth potential $V(x)$ which permits stationary solutions. Then the corresponding stochastic mechanics equation has a solution $\xi_\varphi(t)$ which is a homogeneous Markoff process that is invariant under time reversal and has $\rho(x) = \varphi(x)^2$ as invariant distribution. Moreover the paths of $\xi_\varphi(t)$ are continuous and do not cross the hypersurface $\varphi(x) = 0$, and the semigroup generated by $\xi_\varphi(t)$ is a heat equation semigroup with infinitesimal generator given by

$$-\frac{1}{2} \Delta_\varphi + (V - \lambda),$$

where Δ_φ is the Laplacian with Dirichlet boundary conditions on the hypersurface $\varphi(x) = 0$.

Remark: It follows from this theorem that in the stationary case for higher eigenvalues the stochastic mechanics equation has several solutions, namely those obtained by starting the process in one or some of the domains given by the hypersurface $\varphi(x) = 0$. One may ask the question whether the solution is unique in each of the connected domains Λ_{α} given by the hypersurface $\varphi(x) = 0$. We are able to prove this only in the one dimensional case. The proof goes by explicit examination of all self adjoint extentions of (15) defined on all smooth functions which are zero near the endpoints of the interval Λ_{α} determined by two consecutive zeros of $\varphi(x)$. By using the fact that all such extentions are given by self adjoint boundary conditions, it suffices then to show by a simple calculation that the Dirichlet boundary condition is the only one which has $\varphi(x)$ as an eigenfunction.

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