

## STOCHASTIC MECHANICS, NON-LOCAL POTENTIALS AND JUMP PROCESSES

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An extension of stochastic mechanics which allows for non-local potentials is described. It leads, in general, to integro-differential equations for the probability density and to a stochastic differential equation involving both diffusion and jump processes. A study of non-local potentials of convolution type is carried out in this framework. A simple stochastic description of rotons is obtained.

Some years ago Nelson [1] proposed a formulation of quantum mechanics based on the theory of Markov processes in real time. Stochastic mechanics, as this formulation came to be known, has since been extended and reviewed by several authors [2–4].

At first, the stochastic mechanics formulation of quantum mechanics generated some controversy [5,6]. For one thing the conservative diffusions that appear in stochastic mechanics are very different from those in the familiar dissipative Langevin equation. The mathematical problems raised, in particular, by the singular coefficients in the stochastic differential equations associated to quantum excited states have only recently been clarified [7,8].

The other class of questions raised by stochastic mechanics stem from the desire to interpret quantum mechanics in classical terms which, in my opinion, is a most unrewarding endeavour. In fact, although Nelson's equations are mathematically equivalent to Schrödinger's and one can even derive the excited energy levels from the relaxation times of the ground state process, the process itself does not seem to be directly accessible to observation. For example [4], "... We cannot in fact measure the correlation between the values of the process at different times  $t_1$  and  $t_2$  because any attempt to localize the particle changes the velocity field  $b$ . Therefore after the measurement at  $t_1$  we have a different process."

Nevertheless, the mathematical equivalence of Nelson's and Schrödinger equations enlarges the over-

lap between probability theory and quantum mechanics, making new probabilistic techniques available to the latter. For example the non-linear stochastic mechanics singular perturbation problem associated to tunnelling in the semiclassical limit [9] turns out to be less difficult than the corresponding one for the Schrödinger equation. This is probably true in general for all effects that, having an essential singularity at  $\hbar \rightarrow 0$  or  $g \rightarrow 0$  ( $g$  is the coupling constant), cannot be approached by perturbation theory of the linear Schrödinger equation. The technique that, in this case, is brought to quantum mechanics is the theory of small random perturbations of dynamical systems [10].

Stochastic mechanics provides also a new setting for (real time) stochastic simulation methods in lattice systems [11], excited states being then obtained by the technique of exit times [11,12].

Stochastic mechanics does not provide a new interpretation of quantum mechanics, but in the fact that it is a new set of mathematically equivalent equations of the same theory (which can be dealt with by new techniques) lies its main interest.

Recently I have pointed out [13] that the occurrence of non-local potentials in the Schrödinger equation requires a modification of the usual stochastic mechanics equations. In this paper after reviewing briefly the extended equations for the probability density, the drift and the non-local kernel, one discusses the processes and stochastic differential equations

associated to the stochastic mechanics description of non-local potential effects. One concentrates mostly on non-local potentials which lead to mixed diffusion and jump processes <sup>+1</sup> (in configuration space).

From the Schrödinger equation

$$i\hbar \partial\psi/\partial t = -(\hbar^2/2m)\Delta\psi + V\psi, \quad (1)$$

and its adjoint one obtains the following equation for the probability density  $\rho(x, t) = |\psi(x, t)|^2$

$$\frac{\partial\rho}{\partial t} = -\nabla(b\rho) + \nu\Delta\rho + \text{Im} \int \Sigma(x, y)\rho(y, t) d^n y, \quad (2)$$

where  $\nu = \hbar/2m$  and

$$b = (\hbar/m)\nabla \ln|\psi| + (\hbar/m)\nabla \arg \psi = u + v, \quad (3)$$

$$(V\psi)(x) = \int V(x, y)\psi(y) d^n y,$$

$$V(x, y) = V^*(y, x), \quad (4)$$

$$\Sigma(x, y) = (2/\hbar)\psi^*(x, t)V(x, y)[\psi^*(y, t)]^{-1}. \quad (5)$$

Once a solution  $\psi(x, t)$  of the Schrödinger equation is known, the drift  $b$  and the kernel  $\Sigma(x, y)$  are completely defined. Conversely, interpreting (2) as the density equation of a stochastic process with  $u, v$ , and  $\Sigma$  specified by its equations of motion one obtains the point of view of stochastic mechanics. The equations of motion for  $u, v$  and  $\Sigma$  are

$$\begin{aligned} \dot{u} = & -(\hbar/2m)\nabla_x(\nabla_x v) - \nabla_x(uv) \\ & - (\hbar/2m) \text{Im} \nabla_x \int \Sigma(y, x) d^n y, \end{aligned}$$

$$\begin{aligned} \dot{v} = & \frac{1}{2} \nabla_x(u^2 - v^2) + (\hbar/2m)\nabla_x(\nabla_x u) \\ & - (\hbar/2m) \text{Re} \nabla_x \int \Sigma(y, x) d^n y, \end{aligned}$$

$$\begin{aligned} \dot{\Sigma}(x, y) = & \Sigma(x, y) \left[ \left( -\frac{m}{\hbar}uv(x) - \frac{1}{2} \nabla v(x) \right. \right. \\ & - (im/2\hbar)[u^2(x) - v^2(x)] - \frac{1}{2} i \nabla u(x) \\ & \left. \left. + \frac{1}{2} i \int \Sigma(z, x) d^n z \right) - \{x \leftrightarrow y\} \right]. \end{aligned}$$

If the potential is a local (multiplicative) operator

<sup>+1</sup> Jump processes have already been used by several authors [14–16] to describe quantum dynamics in momentum space. In this paper one considers always stochastic processes in configuration space and the most interesting situations turn out to involve both diffusion and jumping.

$V(x, y) = V(x)\delta(x - y)$ , then  $\Sigma_M(x, y) = (2/\hbar)V(x) \times \delta(x - y)$ ,  $\dot{\Sigma}_M(x, y) = \text{Im} \Sigma_M(x, y) = 0$ . Otherwise, in the non-local case, the kernel  $\Sigma$  has non-trivial dynamics.

In the local case ( $\text{Im} \Sigma_M = 0$ ) the eq. (2) reduces to a Fokker–Planck equation. This in turn is related to a (Langevin) equation for a diffusion process,

$$dx = b dt + \sqrt{\hbar/m} dW, \quad (6)$$

$W$  being a Wiener process normalized to  $\langle dW dW \rangle = dt$ .

There is an important class of non-multiplicative potentials which also lead to diffusion processes. This is the class of Sturm–Liouville potentials,

$$V_{SL} = -K^{ij}(x) \frac{\partial^2}{\partial x^i \partial x^j} - \frac{\partial K^{ij}(x)}{\partial x^i} \frac{\partial}{\partial x^j} + U(x).$$

They also lead [13] to a density equation of the Fokker–Planck type

$$\partial\rho/\partial t = -\partial_i[b^i(x)\rho] + \partial_i[\nu^{ij}(x)\partial_j\rho], \quad (7)$$

where now the diffusion coefficient is position dependent. In the corresponding stochastic differential equations care should therefore be taken in distinguishing between Ito's and Stratonovich's interpretation of stochastic integrals.

Here however, one wants to concentrate on non-local potentials which lead to processes that are not pure diffusions. The examples to be studied will be taken from the class of potentials of convolution type.

Consider a non-local operator of the convolution type ( $V(x, y) = V(x - y)$ )

$$(V\psi)(x) = \int V(x - y)\psi(y) d^n y. \quad (8)$$

The potential being a symmetric operator ( $V(x - y) = V^*(y - x)$ ), one may rewrite (8) as

$$(V\psi)(x) = \frac{1}{2} \int [V(\eta)\psi(x - \eta) + V^*(\eta)\psi(x + \eta)] d^n \eta, \quad (9)$$

i.e. the convolution potential is a superposition of symmetric translation operators. This decomposition suggests the study of a Schrödinger equation with a single translation potential. Choosing one of the coordinate axes along the translation direction, the non-trivial part of the dynamics becomes a one-dimensional problem.

$$\begin{aligned}
 & -(\hbar^2/2m) d^2\psi(x)/dx^2 + \lambda\psi(x+a) + \lambda^* \psi(x-a) \\
 & = E' \psi(x) .
 \end{aligned} \tag{10}$$

Rewrite (10) as

$$\begin{aligned}
 & -(\hbar^2/2m) d^2\psi(x)/dx^2 + \lambda[\psi(x+a) - \psi(x)] \\
 & + \lambda^* [\psi(x-a) - \psi(x)] = E\psi(x) .
 \end{aligned} \tag{11}$$

Using Fourier transforms and defining  $\lambda = |\lambda| \exp(i\theta)$  one concludes that  $\exp(ikx)$  is a (generalized) eigenvector of (11) with eigenvalue

$$E_k = \hbar^2 k^2 / 2m + 2|\lambda| [\cos(ka + \theta) - \cos \theta] . \tag{12a}$$

The dispersion relation (12a) has roton-like features in the sense that  $E_k$  has a local minimum at  $k \neq 0$ , provided  $|\lambda|$  is such that the equation

$$(\hbar^2/2ma^2|\lambda|)x = \sin(x + \theta)$$

has non-trivial solutions.

Similar results hold for the general case  $H = (\hbar^2/2m)\Delta + V$  with  $V$  defined in (9). The plane wave  $\exp[i(\mathbf{k} \cdot \mathbf{x} - E_k t)]$  is a (generalized) eigenvector with energy

$$E_k = \frac{\hbar^2 |\mathbf{k}|^2}{2m} + \int \text{Re}\{V(\boldsymbol{\eta}) \exp(-i\mathbf{k} \cdot \boldsymbol{\eta})\} d^n \boldsymbol{\eta} . \tag{12b}$$

Returning now to the one-dimensional case (11), one wants to find out which stochastic processes are associated to the solutions of the Schrödinger equation with symmetric translation potential. For a plane wave  $\exp[i(kx - E_k t)]$  the drift and the non-local kernel obtained from eqs. (3) and (5) are

$$b = \hbar k / m , \tag{13}$$

$$\text{Im } \Sigma(x, y) = \alpha [\delta(x - y + a) - \delta(x - y - a)] , \tag{14}$$

the coefficient  $\alpha$  being (for a plane wave)

$$\alpha_1 = (2|\lambda|/\hbar) \sin(ka + \theta) . \tag{15}$$

The equation of motion for the probability density (eq. (2)) becomes

$$\begin{aligned}
 \frac{\partial \rho(x, t)}{\partial t} & = -\frac{\hbar k}{m} \frac{\partial \rho(x, t)}{\partial x} + \frac{\hbar}{2m} \frac{\partial^2 \rho(x, t)}{\partial x^2} \\
 & + \alpha [\rho(x + a, t) - \rho(x - a, t)] .
 \end{aligned} \tag{16}$$

Taking the Fourier transform an equation is obtained

for the characteristic function of the process

$$\begin{aligned}
 & dC(u, t)/dt \\
 & = [i(\hbar k/m)u - (\hbar/2m)u^2 - 2i\alpha \sin ua] C(u, t) ,
 \end{aligned} \tag{17}$$

where

$$C(u, t) = \int e^{iux} \rho(x, t) dx = E e^{iux(t)} .$$

The solution of (17) is

$$C(u, t) = C_D(u, t) C_P(u, t) C_{\bar{P}}(u, t) ,$$

where

$$C_D(u, t) = \exp\{[i(k\hbar/m)u - (\hbar/2m)u^2]t\} , \tag{18a}$$

$$C_P(u, t) = \exp\{t|\alpha| [\exp(-iuea) - 1]\} , \tag{18b}$$

$$C_{\bar{P}}(u, t) = f(u) \exp\{-t|\alpha| [\exp(iuea) - 1]\} , \tag{18c}$$

$\epsilon = \text{sign}(\sin(ka + \theta))$  and  $f(u)$  is a function of  $u$  to be specified later on.

$C_D$  is the characteristic function of a diffusion process with coefficient  $\hbar/2m$  and drift  $\hbar k/m$ .  $C_P$  is the characteristic function of a Poisson process with jump size  $-ea$  and coefficient  $|\alpha|$ .

For an appropriate choice of  $f(u)$ ,  $C_{\bar{P}}$  is the characteristic function of a time reversed Poisson process with jump size  $-ea$ . This should be defined with care because a time-reversed process depends not only on the transition functions of the direct process but also on the choice of a particular initial density [17].

Consider a Poisson process with jumps  $+ea$  starting at  $-\epsilon X$  at time  $-T$ . Then the density for the time-reversed process is

$$\begin{aligned}
 \rho_{\bar{P}}(x, t) & = \exp[-|\alpha|(T-t)] \\
 & \times \sum_{n=0}^{\infty} \frac{|\alpha|^n (T-t)^n}{n!} \delta(x + \epsilon X - n\epsilon a) ,
 \end{aligned} \tag{19}$$

which obeys the equation

$$\partial \rho_{\bar{P}}(x, t) / \partial t = |\alpha| \rho_{\bar{P}}(x, t) - |\alpha| \rho_{\bar{P}}(x - \epsilon a, t) .$$

The process with density  $\rho_{\bar{P}}$  is defined in  $t \in (-\infty, T]$  and  $x \in [-\epsilon X, \epsilon\infty)$ . The characteristic function is as in (18c) with

$$f(u) = \exp\{-iueX + |\alpha|T[\exp(iuea) - 1]\} .$$

The transition functions  $Q(t_0, x_0; t, x)$  of the time-

reversed process  $\bar{P}$  are obtained from [17]

$$Q(t, y; s, A) = \left( \int dx \rho_P(x, s) I_A(x) P(s, x; t, y) \right) \times \left( \int dx \rho_P(x, s) P(s, x; t, y) \right)^{-1},$$

where  $\rho_P$  and  $P(\ ; \ )$  are the density and transition functions of a direct Poisson process and  $I_A(x)$  is the indicator function of the set A. Then,

$$Q(t_0, x_0; t, x) = \frac{(\sigma + \xi)!}{\sigma! \xi!} \frac{(t - t_0)^\xi (T - t)^\sigma}{(T - t_0)^{\sigma + \xi}},$$

where  $\xi = \epsilon(x_0 - x)/a$  and  $\sigma = \epsilon(x - X)/a$ .

Unlike the transition function for the direct Poisson process  $P(t_0, x_0; t, x)$

$$P(t_0, x_0; t, x) = \frac{|\alpha|^\xi (t - t_0)^\xi}{\xi!} \exp[-|\alpha|(t - t_0)],$$

the transition function  $Q(t_0, x_0; t, x)$  for the time-reversed process depends on the density parameters  $X$  and  $T$ . Besides the time-reversed process is only defined up to the time  $T$ , all probability being then concentrated at the point  $-eX$ . For practical purposes (numerical solution of stochastic differential equations, for example) it is convenient to choose a density distribution with large  $T$  and  $X$  parameters. Then  $Q(t_0, x_0; t, x)$  becomes

$$Q(t_0, x_0; t, x) \approx \frac{(t - t_0)^\xi}{\xi!} \left( \frac{1 - t/T}{1 - t_0/T} \right)^{X/a} \left( \frac{X/a}{T} \right)^\xi. \tag{20}$$

In the limit  $T, X \rightarrow \infty$  with  $|\alpha|aT = X$  the right-hand side of (20) yields

$$\frac{|\alpha|^\xi (t - t_0)^\xi}{\xi!} \exp[-|\alpha|(t - t_0)], \tag{21}$$

i.e. for this limiting choice of initial density the transition functions of the time-reversed process are identical to those of a direct Poisson process. (The relation  $|\alpha|aT = X$  is the condition that, for the direct process, maximizes the transition probabilities from  $-eX$  at  $t = T$  to the neighbourhood of  $x = 0$  at small  $t$ ).

Having identified the nature of the processes one

may now write the stochastic differential equation which corresponds to the density of eq. (16).

$$x(t) = x(t_0) + \int_{t_0}^t \frac{\hbar k}{m} ds + (\hbar/m)^{1/2} \int_{t_0}^t dW(s) + \int_{t_0}^t dP_{|\alpha|, -\epsilon a}(s) + \int_{t_0}^t d\bar{P}_{|\alpha|, -\epsilon a}(s), \tag{22}$$

The third term is an (Ito) integral over a Wiener process of unit variance and the last two terms denote integration with respect to a Poisson and a time-reversed Poisson process [18,19] with coefficients  $|\alpha|$  and jump  $-\epsilon a$ .

The drift  $b$  and the jump coefficient  $\alpha_1$  in (13)–(15) were derived for a plane wave state. For a wave packet

$$\psi(x, t) = \int F(q) \exp[i(qx - E_q t)] dq,$$

with Fourier transform  $F(q)$  strongly peaked around  $k$  the drift computed from (3) can still be approximated by  $\hbar k/m$ . For the non-local kernel

$$\text{Im } \Sigma(x, y) = (2/\hbar)$$

$$\times \text{Im} \left\{ \lambda \left[ \frac{\psi^*(x, t) \psi(x + a, t)}{\rho(x + a, t)} \delta(x - y + a) - \frac{\psi^*(x - a, t) \psi(x, t)}{\rho(x - a, t)} \delta(x - y - a) \right] \right\},$$

the  $k$  peaking hypothesis is not very helpful and the computation of the coefficients of the delta functions is more delicate. This can be seen, for example, by considering the small  $a$  limit, where the order  $a$  contributions from the first and second terms to the density equation cancel each other. The easiest way to fix the jumping coefficient for wave packet propagation is to adjust it in such a way that the mean displacement of the process coincides with the group velocity obtained from the dispersion relation (12a). From (16) or (22) one obtains for the mean displacement

$$\langle x(t) \rangle = (\hbar k/m - 2a\alpha) t.$$

Comparing with the group velocity  $(1/\hbar) \partial E_k / \partial K$  one obtains (for wave packet propagation)

$$\alpha_2 = (|\lambda|/\hbar) \sin(ka + \theta).$$

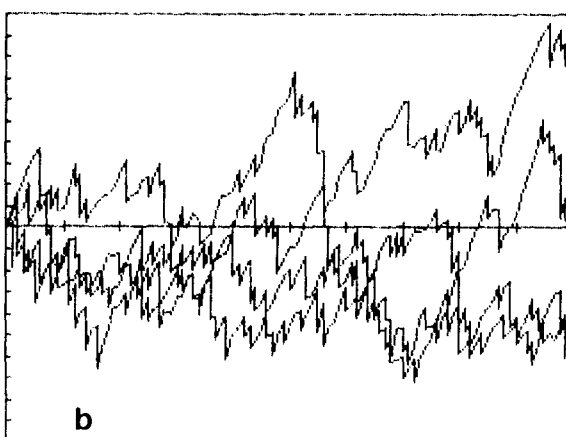
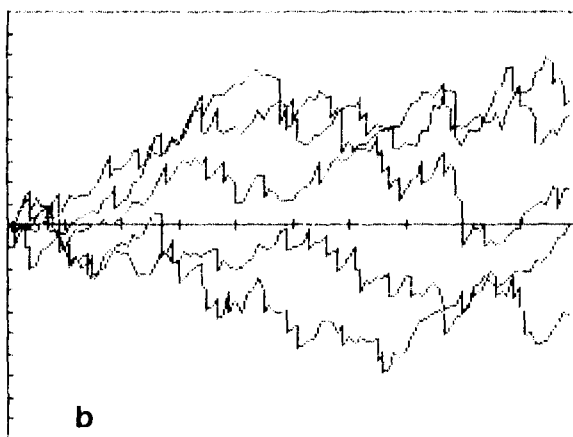
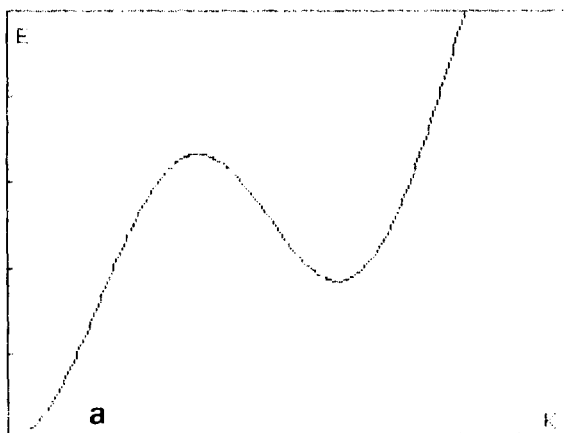
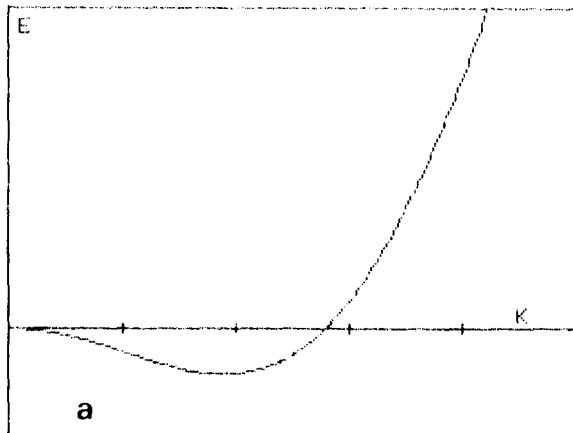


Fig. 1. (a) Dispersion relation for  $\hbar = m = a = 1$  and  $\lambda = 1$ . (b) Sample paths for  $k = 1.895$ .

Fig. 2. (a) Dispersion relation for  $\hbar = m = a = 1$  and  $\lambda = -7$ . (b) Sample paths for  $k = 5.8519$ .

Figs. 1a and 2a display the dispersion relations for  $|\lambda| = 1, \theta = 0$ ; and  $|\lambda| = 7, \theta = \pi$ . In figs. 1b and 2b one sees a few sample paths for the wave packet process at  $k = 1.895$  and  $k = 5.8519$  respectively, i.e. at the non-trivial minima of  $E_k$ . In these (roton) sample paths one sees how cancellation in the average of diffusion and jumping leads to a vanishing mean displacement.

These results can be extended to the case of a general convolution potential defined by (8), (9) with dispersion relation (12b). The corresponding process is a diffusion with drift  $\hbar k/m$  plus a jumping part which is a superposition of Poisson processes defined by the characteristic functions

$$C_P(u, t) = \exp\left(t|\alpha_3| \int d^n \eta \mu(\eta) \times \{\exp[-iu\eta\epsilon(\eta)] - 1\}\right),$$

$$C_{\bar{P}}(u, t) = \exp\left((T-t)|\alpha_3| \int d^n \eta \{-iuX\epsilon(\eta) + \mu(\eta)\{\exp[iu\eta\epsilon(\eta)] - 1\}\}\right),$$

where

$$\alpha_3 = \frac{1}{2\hbar} \int d^n \eta |V(\eta)| |\sin[\mathbf{k} \cdot \boldsymbol{\eta} - \theta(\eta)]|,$$

$$\epsilon(\eta) = \text{sign}(\sin[\mathbf{k} \cdot \boldsymbol{\eta} - \theta(\eta)]),$$

$$\mu(\eta) = (2|\alpha_3|\hbar)^{-1} |V(\eta)| |\sin[\mathbf{k} \cdot \boldsymbol{\eta} - \theta(\eta)]|,$$

$$V(\eta) = |V(\eta)| \exp[i\theta(\eta)].$$

The balance of diffusion and jumping leading to roton effects is an interesting consequence of translation potentials (or convolution potentials in general). If the space where the jumping takes place is compact (an angular variable, for example) the situation is somewhat different. Here one considers only the simplest situation where the potential

$$(V\psi)(x) = V(r)\psi(x) + \lambda\psi(R_\beta x) + \lambda^*\psi(R_\beta^{-1}x) \\ - 2 \operatorname{Re} \lambda \psi(x)$$

contains a radial part plus a symmetric rotation of  $\beta$  around a fixed axis. Choosing this one as the angular momentum quantization axis and writing the wavefunction as

$$\psi(x) = F(r) Y_{lm}(\Omega), \quad \lambda = |\lambda| e^{i\theta},$$

one obtains

$$-\frac{\hbar^2}{2m} \left( \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{l(l+1)}{r^2} \right) + V(r) \\ + 2|\lambda| [\cos(m\beta + \theta) - \cos \theta] F(r) = EF(r).$$

This implies that the  $(nl)$  levels will have an (anomalous) splitting

$$E = E_{nl} + 2|\lambda| [\cos(m\beta + \theta) - \cos \theta].$$

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