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STOCHASTIC MECHANICS AT POSITIVE TEMPERATURE

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The problem of describing quantum thermal processes by stochastic differential equations is reviewed. Extensions to previous approaches are proposed In particular, a general way is found to construct the drift of the thermal process directly from the interaction potential.

The stochastic mechanics formulation of quantum mechanics, introduced by Fényes and Nelson [1,2] and extended by other authors [3–5], provides a set of equations, mathematically equivalent to the Schrödinger equation, which can be dealt with by probabilistic techniques. Carrying over new tools to quantum mechanics, it seems particularly promising in situations not amenable to perturbation theory of the Schrödinger equation. Examples are the semiclassical limit of tunnelling [6] and $\exp(-\lambda/g^2)$ dependent mass gaps in lattice theories [7].

The extension of stochastic mechanics to nonzero temperature was discussed by a few authors [8–11], leading to several definitions of the thermal process. The main problem remaining in the applications of thermal stochastic mechanics lies in the fact that, except in cases where either the exact spectrum or a good set of coherent states are known, the process is not easily amenable to practical computation. In particular for numerical simulation methods, it would be desirable to have a way to generate the drift of the thermal process directly from the potential, without explicit knowledge of the nature of the spectrum.

After reviewing briefly the approaches of Guerra and Loffredo [10] and Ruggiero and Zannetti [11], and pointing out some of their limitations and possible extensions, an equation will be derived which, by evolution from the infinite temperature regime, defines the drift at any finite temperature. For definiteness let $\{\psi_n\}$ be a complete orthonormal set of solutions to the Schrödinger equation

$$i\hbar\partial_t\psi = -(\hbar^2/2m)\Delta\psi + V(x)\psi. \tag{1}$$

The quantum equilibrium state at temperature T is described by the density matrix ρ

$$\rho\phi = Z^{-1}(\beta)\sum_n e^{-\beta E_n}\psi_n(\psi_n, \phi). \tag{2}$$

In stochastic mechanics, to each state ψ_n one associates a stochastic process $x_n(t)$ solution to the stochastic differential equation

$$dx_n(t) = b_n\,dt + \sqrt{\hbar/m}\;dW(t), \tag{3}$$

where $\langle dW(t)\rangle = 0$, $\langle dW(t)\,dW(t)\rangle = dt$, $b_n = u_n + v_n$,

$$u_n(x, t) = (\hbar/m)\nabla\,\ln|\psi_n(x, t)|, \tag{4a}$$

$$v_n(x, t) = (\hbar/m)\nabla\,\arg\psi_n(x, t). \tag{4b}$$

To the thermal mixture state at temperature T corresponding to the density matrix ρ [eq. (2)], Guerra and Loffredo [10] associate a stochastic process $x(t)$ which they define through the generic average

$$\langle F(x(t_1)\ldots x(t_s))\rangle$$
$$= Z^{-1}\sum_n e^{-\beta E_n}\langle F(x_n(t_1)\ldots x_n(t_s))\rangle. \tag{5}$$

One may actually give a more explicit characterization of the thermal process. From the position probability density

$$\rho(x, t) = \mathrm{Tr}(|x\rangle\langle x|\rho)$$
$$= Z^{-1}(\beta)\sum_n e^{-\beta E_n}\rho_n(x, t), \qquad (6)$$

where $\rho_n(x, t) = |\psi_n(x, t)|^2$ and eq. (3), one may compute

$$d\langle f(x(t))\rangle = \int dx\, f(x)\partial_t\rho(x, t)\, dt$$

for an arbitrary function and obtain

$$dx(t) = \frac{\sum_n e^{-\beta E_n}\rho_n b_n}{\sum_n e^{-\beta E_n}\rho_n}\, dt + \sqrt{\hbar/m}\, dW(t). \qquad (7)$$

Using the decomposition $b_n = u_n + v_n$, the drift of the thermal process may be separated into its osmotic and current velocity parts. They are written in the following form which will be useful later on:

$$u_\beta(x, t) = (\hbar/2m)\nabla_x \ln \rho(x, t)$$
$$= \frac{\hbar}{2m}\frac{\sum_n e^{-\beta E_n}(\psi_n^*\nabla\psi_n + \psi_n\nabla\psi_n^*)}{\sum_n e^{-\beta E_n}\rho_n},$$
$$(8a)$$

$$v_\beta(x, t) = \frac{\sum_n e^{-\beta E_n}\rho_n v_n}{\sum_n e^{-\beta E_n}\rho_n}$$
$$= \frac{\hbar}{2im}\frac{\sum_n e^{-\beta E_n}(\psi_n^*\nabla\psi_n - \psi_n\nabla\psi_n^*)}{\sum_n e^{-\beta E_n}\rho_n}.$$
$$(8b)$$

There is another way to look at the thermal process which, although leading to the same observable average values, would correspond to different sample paths. Instead of the process with a fixed average drift function, as in eq. (7), one might consider a stochastic drift and define the thermal process as the solution $x'(t)$ of the stochastic equation

$$dx'(t) = b_{n,x}(t)\, dt + \sqrt{\hbar/m}\, dW(t), \qquad (9)$$

where now $b_{n,x}(t)$ is also a stochastic process with values in the space of functions $\{b_n(x, t) = u_n(x,t) + v_n(x,t)\}$ and probability law $p(n, x, t) = \sum_n e^{-\beta E_n}\rho_n b_n/\sum_n e^{-\beta E_n}\rho_n$.

The finite temperature formulations specified by eqs. (5) or (7) and (9) require either global knowledge on the space of solutions to the Schrödinger equation or, alternatively, some indirect way to find the thermal drift functions (see below). Guerra and Loffredo [10] show that for the harmonic oscillator the summation in (5) becomes simpler when one uses a coherent state basis. In any case, summing or integrating over an infinite set of states seems adequate only when either the exact solutions to the Schrödinger equation are known or they can be approximated by some set of generalized coherent states. Such infinite sums are certainly difficult to handle when numerical methods are called for.

A technique that does not require a priori knowledge on the space of solutions was proposed by Ruggiero and Zannetti [11]. Considering quantum processes $x(t)$ which are decomposable into a classical $q(t)$ plus a ground state quantum motion $\xi(t)$, they write the multivariable process

$$dp(t) = -(\partial H/\partial q)\, dt, \qquad (10a)$$
$$dq(t) = (\partial H/\partial p)\, dt, \qquad (10b)$$
$$dx(t) = [\partial H/\partial p + b_0(x - q, t)]\, dt$$
$$+ \sqrt{\hbar/m}\, dW(t), \qquad (10c)$$

where $b_0(\xi, t) = u_0 + v_0$ is obtained from the ground state ψ_0 as in eqs. (4).

To construct the thermal process, Ruggiero and Zannetti connect the system to a heat bath with which it interacts through the dynamics of the $p(t)$, $q(t)$ variables. Hence the first equation in the set (10) is replaced by

$$dp(t) = (\partial H/\partial q)\, dt - \gamma p\, dt + D^{1/2}\, d\eta(t), \qquad (11)$$

where $\eta(t)$ is a Wiener process uncorrelated to the one in (10c), and γ and D are related in such a way that a balance between energy absorption from the random driving force and dissipative transfer to the bath is obtained at temperature T. Eqs. (10b) and (10c) with the new eq. (11) describe the thermal process.

This approach will lead to a correct quantum behaviour only if $b' = \partial H/\partial p + b_0(x - q, t)$ is a quantum drift, i.e., if, for each pair $(p(t), q(t))$,

there is a state $\psi_{p,q}$ such that $b' = (\hbar/m) \times \nabla\{\ln|\psi_{p,q}| + \arg \psi_{p,q}\}$. This holds for quadratic potentials but is not true in general, meaning that a generic quantum motion cannot be simply decomposed into classical plus ground state motion. This is the reason why, in order to deal with anharmonic interactions, Ruggiero and Zannetti actually replace the potential by an effective harmonic one, in a self-consistent approximation.

The idea of defining the thermal state as a multivariable process can, however, be formulated in a way that does not assume the particular $x(t) = q(t) + \xi(t)$ decomposition of Ruggiero and Zannetti. In stochastic mechanics, a quantum process can be completely defined (without any reference to a Schrödinger equation) as a solution to the following set of equations:

$$dv = \left[\tfrac{1}{2}\nabla(u^2 - v^2) + (\hbar/2m)\nabla(\nabla \cdot u)\right.$$
$$\left. - m^{-1}\nabla V(x)\right] dt, \quad (12a)$$

$$du = \left[-(\hbar/2m)\nabla(\nabla \cdot v) - \nabla(u \cdot v)\right] dt, \quad (12b)$$

$$dx = (u + v) \, dt + (\hbar/m)^{1/2} \, dW(t). \quad (12c)$$

The osmotic velocity u depends only on the density of the process [see eq. (8a)], and its role is to damp the fluctuations. Interaction with external sources [the potential $V(x)$ for example] is carried by the current velocity v. The equation of motion (12a) for v is equivalent to a Newton law in the mean

$$ma = -\nabla V(x), \quad (13)$$

where $a = \tfrac{1}{2}(D_+D_- + D_-D_+)x(t)$ with the mean forward (backward) derivative D_+ (D_-) being defined by

$$D_\pm f(x, t) = \lim_{\Delta t \to 0} E\left\{ \pm \left[f(x_{t \pm \Delta t}, t \pm \Delta t)\right.\right.$$
$$\left.\left. - f(x_t, t)\right]/\Delta t \,|\, x_t = x \right\}.$$

Equivalence of (13) and (12a) is easily proved by noticing that $D_\pm x(t) = v \pm u$.

The equivalence of (12a) to a Newton law in the mean suggests a way to construct a thermal process. To describe the interaction of the system with the thermal bath, one replaces the Newton

law (13) by

$$ma = -\nabla V(x) - \gamma mv + D^{1/2} \, d\eta/dt. \quad (14)$$

From (14), one now obtains

$$dv = \left[\tfrac{1}{2}\nabla(u^2 - v^2) + (\hbar/2m)\nabla(\nabla \cdot u)\right.$$
$$\left. - m^{-1}\nabla V(x) - \gamma v\right] dt$$
$$+ (D^{1/2}/m) \, d\eta(t). \quad (15)$$

Eqs. (12b), (12c) and (15) would then define the quantum thermal process.

Although, in principle, this way of defining the thermal process is more general than that of Ruggiero and Zannetti, the resulting equations are not very easy to use; in particular, the stability of numerical solutions is hard to control. For this reason, I now turn to an attempt to construct the average thermal drift for the stochastic equation (7) directly from the potential. For this purpose, one defines the quantities

$$r(z, x, \beta) = \sum_n e^{-\beta E_n}\psi_n(z, t)\psi_n^*(x, t), \quad (16)$$

$$u(z, x, \beta) = \frac{\hbar}{2m}\frac{1}{r(z, x, \beta)}$$
$$\times (\nabla_x + \nabla_z)r(z, x, \beta), \quad (17)$$

$$v(z, x, \beta) = \frac{\hbar}{2im}\frac{1}{r(z, x, \beta)}$$
$$\times (\nabla_z - \nabla_x)r(z, x, \beta). \quad (18)$$

From eqs. (8), it is clear that

$$\lim_{z \to x} u(z, x, \beta) = u_\beta(x, t), \quad (19a)$$

$$\lim_{z \to x} v(z, x, \beta) = v_\beta(x, t). \quad (19b)$$

The reason for defining these quantities is that their β-derivatives can be represented as differential expressions of the same quantities.

$$(\partial/\partial\beta)u^j(z, x, \beta) = -(\hbar/2m)\nabla_z^j V(z)$$
$$+ (\hbar^2/2m)\Delta_z u^j + \hbar(\nabla_z u^j) \cdot (u + iv), \quad (20)$$

$$(\partial/\partial\beta)iv^j(z, x, \beta) = -(\hbar/2m)\nabla_z^j V(z)$$
$$+ (\hbar^2/2m)\Delta_z iv^j + \hbar(\nabla_z iv^j) \cdot (u + iv). \quad (21)$$

Now eqs. (20) and (21) are interpreted as evolu-

tion equations (in β) and the quantities $u(z, x, \beta)$ and $v(z, x, \beta)$ may be obtained by integration from the neighbourhood of the infinite temperature limit ($\beta = 0$). In this limit, one has in leading order

$$u(z, x, \beta) \approx 0, \qquad (22a)$$

$$iv(z, x, \beta) \approx (\hbar/\beta)(x - z), \qquad (22b)$$

which may easily be checked from the fact that dominance of the kinetic energy terms at $T \to \infty$ makes $v(z, x, \beta)$ proportional to $\exp[-(m/2\beta) |z - x|^2]$ in leading order.

By integration from the initial conditions (22) at some small β_0, the quantities $u(z, x, \beta)$ and $v(z, x, \beta)$ may, in principle, be obtained for any β and any smooth potential. The components of the thermal drift are then picked up at the $z \to x$ limit [eqs. (19)]. Before discussing the problems involved in the numerical integration of eqs. (20) and (21), an approximate solution will be obtained which is useful in improving the boundary conditions at small β. Define

$$f(z, x, \beta) = u(z, x, \beta) + iv(z, x, \beta), \qquad (23)$$

which obeys the equation

$$\partial f/\partial \beta = -(\hbar/m)\nabla_z V(z) + (\hbar^2/2m)\Delta_z f + \hbar f \cdot \nabla_z f. \qquad (24)$$

In many cases, f is actually the only quantity of interest, because for isolated systems with real potentials $v(z, x, \beta)$ vanishes in the $z \to x$ limit and

$$\lim_{z \to x} f(z, x, \beta)$$

is the physical drift at inverse temperature β.

For simplicity, I will restrict myself to the one-dimensional case. Assuming the existence of a solution to eq. (24) analytic at $z - x = 0$, one writes

$$f(z, x, \beta) = \sum_{k=0} \frac{A_k(\beta)}{k!} (z - x)^k. \qquad (25)$$

From (24) and (25), one now obtains an (infinite) system of ordinary differential equations in β.

$$\frac{d}{d\beta} A_k(\beta) = -\frac{\hbar}{m} \frac{d^{k+1}V(x)}{dx^{k+1}} + \frac{\hbar^2}{2m} A_{k+2} + \hbar \sum_{\{j+j'=k\}} \binom{k}{j} A_{j+1} A_{j'}. \qquad (26)$$

In general these equations are difficult to solve. However, if the derivatives of the potential $\partial_k V(x)$ above $k = 2$ can be neglected, eqs. (26) imply that, starting from an initial condition where $A_j(\beta_0) = 0$ for $j \geq 2$, then $A_j(\beta) = 0$ for $j \geq 2$ and all β. In this case, the set (26) has only two non-trivial equations which, with the initial condition $[A_0(\beta_0) = 0, \ A_1(\beta_0) = -\hbar/\beta_0]$, lead to the solutions:

$$A_0(\beta) = -\frac{\partial_x V}{\sqrt{m\partial_x^2 V}} \frac{\cosh\left(\hbar\beta\sqrt{m^{-1}\partial_x^2 V}\right) - 1}{\sinh\left(\hbar\beta\sqrt{m^{-1}\partial_x^2 V}\right)},$$

$$\text{if} \quad \partial_x^2 V > 0,$$

$$= \frac{\partial_x V}{\sqrt{m|\partial_x^2 V|}} \frac{\cos\left(\hbar\beta\sqrt{m^{-1}|\partial_x^2 V|}\right) - 1}{\sin\left(\hbar\beta\sqrt{m^{-1}|\partial_x^2 V|}\right)},$$

$$\text{if} \quad \partial_x^2 V < 0,$$

$$= -(\hbar\beta/2m)\partial_x V,$$

$$\text{if} \quad \partial_x^2 V = 0, \qquad (27)$$

$$A_1(\beta) = -\sqrt{m^{-1}\partial_x^2 V} \coth\left(\hbar\beta\sqrt{m^{-1}\partial_x^2 V}\right),$$

$$\text{if} \quad \partial_x^2 V > 0,$$

$$= -\sqrt{m^{-1}|\partial_x^2 V|} \cot g\left(\hbar\beta\sqrt{m^{-1}|\partial_x^2 V|}\right),$$

$$\text{if} \quad \partial_x^2 V < 0,$$

$$= -1/\hbar\beta,$$

$$\text{if} \quad \partial_x^2 V = 0, \qquad (28)$$

where the limit $\beta_0 \to 0$ has been taken.

For anharmonic potentials, these solutions are not expected to hold beyond the region of small β, because as the temperature decreases one needs, at each point x in the integration of eq. (24), detailed information on the local analytic structure of the potential to be able to account for the global behaviour of the lowest-lying eigenstates. However, even for general potentials, the approximate solutions are useful because they supply

improved boundary conditions at small β_0 for the numerical integration of eq. (24).

Numerical integration of eq. (24) is relatively simple. For each point x, one defines initial conditions $f(z, x, \beta_0) = A_0(\beta_0) + A_1(\beta_0)(z - x)^{-1}$ at a mesh of $2N + 1$ points $\{z = x \pm \imath \Delta z; \imath = 0, \ldots, N\}$. After each iteration the outermost points must be dropped, because of the finite difference evaluation of the derivatives. Therefore the integration extends to, at most, $\beta_{max} = N\Delta\beta + \beta_0$.

Being a non-linear relative to the heat equation, eq. (24) needs the same careful treatment to ensure stability of the finite difference scheme. Applying von Neumann's criterion [12] and a local analysis of the Lyapunov exponents, the following conditions are obtained:

$$\Delta\beta < (\Delta z)^2, \tag{29a}$$

$$F\Delta\beta < 2\Delta z, \tag{29b}$$

$$DF(\Delta z)^2 < 1, \tag{29c}$$

where F and DF are upper bounds on the absolute values of the function f and its first derivative. The condition (29a) is a familiar one from the heat equation, whereas (29b) and (29c) are characteristic of the non-linearity. Being obtained from worst-case estimates, these conditions should be taken as order-of-magnitude guides, not as strict inequalities. Taken literally, they would imply that $\beta_{max} \leqslant 2\beta_0$. In fact, with appropriate care on can, in practice, carry the integration to values of β, where the drift is already close to the ground state drift.

The conditions (29b) and (29c) are taken into account, in the integration program, by inspecting at each iteration the absolute values of the function and its derivative and, if at a point K of the mesh they exceed a prescribed bound, all points beyond K are discarded. The integration then proceeds with the remaining inward part of the mesh. In fig. 1 is shown the result of one such integration for the potential $V(x) = x^4 - x^2$, with $\hbar = m = 1$. Only the positive x-axis is shown, the drift being antisymmetric. One sees clearly how the thermal drift reflects the fact that, as the temperature decreases, the average position spread of the particle moves inwards.
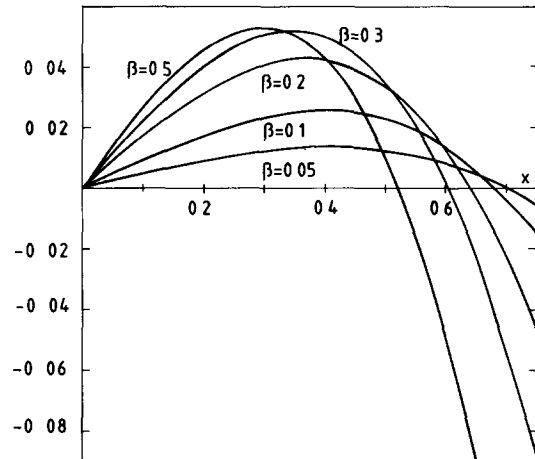

Fig. 1. Thermal drifts at positive temperature for the potential $V(x) = x^4 - x^2$ ($\hbar = m = 1$).

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