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REPLY

Reply to 'Comment on 'Semiclassical Klein–Kramers and Smoluchowski equations for the Brownian motion of a particle in an external potential''

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Abstract
We reply to Tsekov's comments (2007 *J. Phys. A: Math. Theor.* **40** 10945) concerning the semiclassical quantum master equation.

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In his comments Tsekov [1] has discussed the range of the applicability of the semiclassical Smoluchowski equation for the configuration space distribution function $P(x,t) = \int_{-\infty}^{\infty} W(x, p, t)\,\mathrm{d}p$ derived in [2], namely,

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial x}\left\{\frac{P}{\zeta}\frac{\partial V}{\partial x} + \frac{\partial}{\partial x}(D_{\mathrm{eff}}P)\right\}, \tag{1}$$

where $W(x, p, t)$ is the Wigner distribution function in the phase space (x, p); $\zeta = \gamma m$ and $D_{\mathrm{eff}} = D[1 + (\hbar^2\beta^2/12m)V''(x)] + O(\hbar^4)$ have the meaning of friction and diffusion coefficients, respectively; $D = 1/(\zeta\beta)$, $\hbar$ is Planck's constant, m is the mass of the particle and γ is a friction parameter measuring the strength of the coupling to the heat bath. We recall that equation (1) has been obtained by a standard (Kramers) procedure using the approximation of frequency-independent damping from the corresponding semiclassical Klein–Kramers equation for the Wigner function $W(x, p, t)$; this equation to order $\hbar^2$ is

$$\frac{\partial}{\partial t}W + \frac{p}{m}\frac{\partial W}{\partial x} - \frac{\partial V}{\partial x}\frac{\partial W}{\partial p} + \frac{\hbar^2}{24}\frac{\partial^3 V}{\partial x^3}\frac{\partial^3 W}{\partial p^3} + \cdots$$
$$= \gamma\frac{\partial}{\partial p}\left[pW + \frac{m}{\beta}\left\{1 + \frac{\hbar^2\beta^2}{12m}\frac{\partial^2 V}{\partial x^2} + \cdots\right\}\frac{\partial W}{\partial p}\right]. \tag{2}$$

Equation (2) is a partial differential equation for the evolution of the Wigner quasiprobability distribution W akin to the Klein–Kramers equation and in the classical limit reduces to the classical Klein–Kramers equation for the distribution function $W(x, p, t)$ in the phase space

$$\frac{\partial}{\partial t}W + \frac{p}{m}\frac{\partial W}{\partial x} - \frac{\partial V}{\partial x}\frac{\partial W}{\partial p} = \frac{\zeta}{m}\frac{\partial}{\partial p}\left[pW + \frac{m}{\beta}\frac{\partial W}{\partial p}\right]. \tag{3}$$

The main objection of Tsekov [1] is that 'equation (1) does not describe well enough the evolution'. Furthermore, equation (1) predicts that 'the position dispersion σ^2 of the free Brownian particle $[V(x) = 0]$ obeys the classical Einstein law $\sigma^2 = 2Dt$'. From Tsekov's point of view the proof of the incorrect behavior is given in [3], where 'numerical simulations have shown, however, that the front of the Gaussian quantum diffusion advances as $\sigma \sim t^{1/4}$'.

According to Tsekov's quantum theory of thermodynamic relaxation (TQTTR) [4, 5], his 'advanced Smoluchowski' equation

$$\frac{\partial P}{\partial t} = D\frac{\partial}{\partial x}P\frac{\partial}{\partial x}\int_0^\beta \frac{1}{\sqrt{P}}\left\{\hat{H} + 2\frac{\partial}{\partial \beta}\right\}\sqrt{P}\,\mathrm{d}\beta, \tag{4}$$

($\hat{H}$ is the Brownian particle Hamiltonian) describes correctly the evolution of quantum systems. We remark that in the weak coupling limit (treated in [2]) Tsekov's equation (4) predicts for the free Brownian particle (equation (7) of [1])

$$\sigma^2 = 2Dt + \left(\frac{D^2\hbar^2}{4m}\int_0^\beta \frac{1}{D^2}\,\mathrm{d}\beta\right)\ln t + \text{const}. \tag{5}$$

We also remark that according to the TQTTR [5], the corresponding kinetic equation for the classical distribution function $W(x, p, t)$ in the phase space (corresponding to the Klein–Kramers equation (3)) is the last equation on page 70 of [5]; in our notation

$$\frac{\partial}{\partial t}W + \frac{p}{m}\frac{\partial W}{\partial x} - \frac{\partial V}{\partial x}\frac{\partial W}{\partial p} = \frac{\zeta}{m}\frac{\partial}{\partial p}\left[pW + \frac{m}{\beta}\frac{\partial W}{\partial p}\right] + \frac{1}{\zeta}\frac{\partial}{\partial x}\left[W\frac{\partial V}{\partial x} + \frac{1}{\beta}\frac{\partial W}{\partial x}\right]. \tag{6}$$

Finally, if the system is close to equilibrium Tsekov states that one can derive from equation (4)

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial x}\left\{\frac{P}{\zeta}\frac{\partial}{\partial x}V_{\mathrm{eff}} + \frac{\partial}{\partial x}\left[D_{\mathrm{eff}}P\right]\right\}, \tag{7}$$

where $V_{\mathrm{eff}}(x) = V(x) + \frac{\hbar^2\beta}{24m}V''(x) + \cdots$ is an effective potential. This equation is the high-temperature limit of that derived by Ankerhold *et al* [6] and as we have noticed in [2] it is not identical to equation (1).

We first note by way of refutation of the points raised by Tsekov that his 'advanced' equation (4) is *nonlinear*. Thus it cannot in any sense be classified as a Smoluchowski equation which is a *linear* equation. Moreover, both the quantum equation (5) and Tsekov's classical equation (6) exhibit unphysical singular behavior in the limits $t \to 0$ and $\zeta \to 0$, respectively. Furthermore, equation (5) as written makes no physical sense at all as a normalizing time constant is missing in $\ln t$ (we recall that all parameters in the above equation must have the appropriate physical dimensions). Finally the numerical simulations presented by Cerovski *et al* [3] pertain to *anomalous diffusion*, where $\sigma^2 \sim t^\alpha$, and not to the *normal diffusion* treated in [2].

Equation (1) indeed predicts that the position dispersion σ^2 of the free Brownian particle $[V(x) = 0]$ obeys the classical Einstein law $\sigma^2 = 2Dt$ because with $V(x) = 0$, equation (1) coincides with the classical Smoluchowski equation. Moreover, Wigner's formulation of the dynamics of the free particle $[V(x) = 0$ and $\gamma = 0]$ is formally equivalent in all respects to the Liouville equation description of the free particle dynamics as evidenced by the evolution equation for the Wigner quasiprobability distribution W

$$\frac{\partial}{\partial t}W + \frac{p}{m}\frac{\partial W}{\partial x} = 0 \tag{8}$$

which does not depend explicitly on $\hbar$. Now by analogy with the classical kinetic theory, equations (1) and (2) can be considered as a kinetic model (*Stosszahlanzatz*) as we have simply used the extension to the semiclassical case of a heuristic idea originally used by Einstein, Smoluchowski, Langevin and Kramers in order to calculate drift and diffusion coefficients in the classical theory of the Brownian motion. Thus allowing us [2] to understand how quantum effects treated in semiclassical fashion alter the classical Brownian motion in a potential. We emphasize that equations (1) and (2) can be used to describe the evolution of a quantum system in the high-temperature and weak-coupling limits only. We remark in passing as shown in [7], in the noninertial (overdamped) limit, where equation (1) is applicable, that it is in complete agreement with the quantum escape rate theory. In [2] we have obtained equations (1) and (2) in the approximation of *frequency-independent* damping, where the drift and diffusion coefficients are *independent* of the time. In the high-temperature limit, this approximation may be used both in the limits of *weak* and *strong* damping. One would expect that the master equation (2) is a reasonable approximation for the kinetics of a quantum Brownian particle in a potential $V(x)$, when $\beta\hbar\zeta/m \ll 1$. For the range of parameters, where such an approximation is not valid (e.g., throughout the very low-temperature region), other methods should be used.

The quantum Smoluchowski equation (7) is *very similar* but not *identical* to equation (1). We see that equation (7) differs from equation (1) only by the additional term in V_{eff}. However, this difference is important, because the stationary solution of equation (7) in the high-temperature limit is

$$P_A(x) \sim \mathrm{e}^{-\beta V(x)}\left[1 + \frac{\hbar^2\beta^2}{24m}(\beta V'(x)^2 - 3V''(x)) + \cdots\right],$$

which is similar to the coordinate-dependent part of the Wigner phase-space distribution

$$W_{\text{st}}(x, p) = \mathrm{e}^{-\beta\varepsilon(x,p)}\left[1 + \frac{\hbar^2\beta^2}{24m}(\beta V'^2(x) - 3V''(x) + V''(x)(\beta p^2/m)) + \cdots\right],$$

where $\varepsilon(x, p) = p^2/(2m) + V(x)$ resulting from omitting the p^2 term. However, the *true* Wigner equilibrium distribution in configuration space

$$P_{\text{st}}(x)\int_{-\infty}^{\infty} W_{\text{st}}(x, p)\,\mathrm{d}p \sim \mathrm{e}^{-\beta V(x)}\left\{1 + \frac{\hbar^2\beta^2}{24m}\left[\beta V'(x)^2 - 2V''(x)\right] + \cdots\right\} \tag{9}$$

does not coincide with $P_A(x)$ and so *does not satisfy* equation (7). This is an obvious drawback of equation (7). On the other hand, the equilibrium distribution $P_{\text{st}}(x)$ is a stationary solution of equation (1).

In order to explain the anomalous subdiffusion behavior of $\sigma^2 \sim t^\alpha$, the semiclassical Smoluchowski equation (1) for the configuration space distribution function $P(x, t)$ can be readily generalized to anomalous semiclassical diffusion (just as in the classical case [8, 9])

$$\frac{\partial P}{\partial t} = {}_0D_t^{1-\alpha}\frac{\partial}{\partial x}\left\{\frac{P}{\zeta}\frac{\partial V}{\partial x} + \frac{\partial}{\partial x}(D_{\text{eff}}P)\right\}. \tag{10}$$

Here the operator ${}_0D_t^{1-\alpha} \equiv \frac{\partial}{\partial t}\, {}_0D_t^{-\alpha}$ in equation (10) is given by the convolution (the Riemann–Liouville fractional integral definition)

$$ {}_0D_t^{-\alpha} W(x,t) = \frac{1}{\Gamma(\alpha)} \int_0^t \frac{W(x,t')\,\mathrm{d}t'}{(t-t')^{1-\alpha}}, \tag{11} $$

where $\Gamma(z)$ is the gamma function. The physical meaning of the parameter α is the order of the fractional derivative in the fractional differential equation describing the continuum limit of a random walk with a *chaotic* set of waiting times (often known as a fractal time random walk) in contrast to the random walk associated with the normal diffusion where the elementary steps are taken at *uniform* intervals in time. In particular, equation (10) predicts $\sigma^2 \sim t^\alpha$ just as in the classical case [8, 9].

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