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Monitoring the wave function by time continuous position measurement

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New Journal of Physics **12** (2010) 043038 (11pp)


Received 30 November 2009

Published 21 April 2010

Online at <http://www.njp.org/>

doi:10.1088/1367-2630/12/4/043038

Abstract. Motivated by the technical requirements of quantum information processing and nanotechnology, the control of individual quantum systems such as single atoms, ions or even photons has become a highly desirable aim. The monitoring of quantum systems—a direct test and in many cases a prerequisite of their control—has been investigated so far only for certain observables such as the position or momentum of quantum particles. Here, we describe a method to monitor in real time the complete state of a quantum particle with unknown initial state moving in a known potential. The method is based on successively updating an estimate by the results of a continuous position measurement. We demonstrate by numerical simulations that even in a chaotic potential tracking the wave function of a particle is possible, and we show with an example that the monitoring scheme appears to be robust against sudden random perturbations.

 Online supplementary data available from stacks.iop.org/NJP/12/043038/mmedia

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1. Introduction

Monitoring—continuous observation—of a dynamical system in the presence of randomness is not only employed in physics and chemistry, e.g. to survey the motion of comets, the growth of thin layers or the dynamics of chemical reactions. In addition, it is a sub-discipline of robotics and also plays a vital role in other fields such as earth science and aeronautics, with its numerous applications including those in climate observation, the control of robots and vehicles, and remote sensing. Monitoring tasks can be modelled by stochastic processes supported by continuous updates of estimates according to the observed random data—also called stochastic filtering [1]. A special challenge, however, is posed in the realm of quantum physics; the preparation—not to mention monitoring or control—of individual atoms, electrons and photons remained experimentally unattainable for half a century. The theory of quantum monitoring emerged only 20 years ago [2–5]. Now, however, nanotechnology and quantum information processing strongly inspire a mathematical theory of monitoring and control of single quantum degrees of freedom like, e.g., the position of an atom or a nano-object. A more challenging aim is to monitor and control the entire state of individual quantum systems.

In monitoring a quantum system the principal difficulties one encounters lie in the characteristic traits of quantum nature itself: incompatible observables such as position and momentum, as well as an irreversible state change introduced by measurements. Methods have been developed to employ monitoring in order to determine the pre-measurement state [6], for parameter estimation [7], to track oscillations between distinguishable states [8]–[10] and—combined with feedback—for cooling purposes [11] or to reach a targeted state [12]. Moreover, the possibility of state monitoring has been studied for special systems [13, 14]. We will show here that monitoring the position of a single quantum particle promises—via our theory—the monitoring of the full wave function, i.e. the complete state of a particle; we demonstrate its power by numerical simulations. As is always the case in the quantum realm, monitoring will unavoidably alter the original (unmonitored) evolution of the wave function. Strong monitoring ensures a high-fidelity record of the system’s dynamics but has little to do with the evolution of the unmonitored wave function, because of the disturbing influence of the monitoring. Fortunately, in many cases, a suitably small strength of monitoring ensures both a slight change of self-dynamics and—after a certain waiting period—robust fidelity of the record. Here, the length of this period increases with decreasing strength of the monitoring. Needless to say, such

compromise is not due to any weakness in our theory. It is definitely an ultimate necessity enforced by the Heisenberg uncertainty relations.

In the following, the concept of continuous observation is interpreted as the asymptotic limit of dense sequences of unsharp position measurements on a single quantum particle. We describe the inference of its wave function from the sequence of measured position data and then compare the true wave function with its estimate using simulations of quantum particles moving in various potentials. Among them is the Hénon–Heiles potential, which in classical physics implies chaotic behaviour and thus exposes tracking of dynamics to extreme conditions.

2. Monitoring the position

Time-continuous position measurement can be understood as an idealization of a sequence of discrete unsharp position measurements carried out consecutively on a single quantum particle [3]. The notion of unsharp measurement is instrumental here. Such an unsharp measurement of the position \hat{q} can be realized as indirect von Neumann measurement; instead of measuring the particle's position directly, an ancilla system is scattered off the particle and then the ancilla is measured [15]–[19]. The observed results yield limited information on the position \hat{q} of the scatterer as well as less average state change than a projection measurement—both characteristic traits of an unsharp measurement of \hat{q} . In order to realize an unsharp measurement, the ancillas should be interacting weakly with the particle or initially be prepared in a sufficiently non-localized state. In a simple description, a single unsharp measurement of resolution σ collapses the wave function onto a neighbourhood with characteristic extent σ of a random value \bar{q} :

$$\psi(q) \longrightarrow \frac{1}{p(\bar{q})} \sqrt{G_\sigma(q - \bar{q})} \psi(q), \quad (1)$$

where $G_\sigma(q) = (1/\sqrt{2\pi\sigma^2}) \exp(-q^2/2\sigma^2)$ is a central Gaussian function. The random quantity \bar{q} is the measured position that determines the collapse, i.e. the weighted projection, of the wave function. The probability of obtaining the measurement result \bar{q} —which also plays the role of a normalization factor of the post-measurement wave function—reads as

$$p(\bar{q}) = \int G_\sigma(q - \bar{q}) |\psi(q)|^2 dq. \quad (2)$$

As a matter of fact, sharp (direct) von Neumann position measurements are the idealized special case, while unsharp measurements—although not necessarily with the Gaussian profile—are the ones that we encounter in practice and that suit a tractable theory of real-time monitoring of the position of a single quantum particle.

In our discretized model of monitoring a single particle, we assume an unknown initial wave function $\psi_0(q)$ and perform consecutive unsharp position measurements of resolution σ at times $t = \tau, 2\tau, \dots$, respectively, yielding the corresponding sequence \bar{q}_t of measurement outcomes. Between two consecutive unsharp measurements, the wave function evolves according to its Schrödinger equation (self-dynamics).

The resolution σ and the frequency $1/\tau$ of unsharp measurements should be chosen in such a way as to not heavily distort the self-dynamics of the particle. It turns out that the relevant parameter is $\sigma^2\tau$; we call

$$\gamma = \frac{1}{\sigma^2\tau} \quad (3)$$

the strength of position monitoring. The strength of position monitoring γ is related to the average strength of the back action the measurements exert on the system. This can be seen in the continuum limit $\tau \rightarrow 0$ and $\sigma \rightarrow \infty$, such that γ stays finite (cf the [appendix](#)). In the absence of unitary dynamics, the system's density matrix in position representation $\rho(q, q', t) = \langle q | \hat{\rho}(t) | q' \rangle$ would evolve due to a continuous position measurement in the non-selective regime according to the Master equation [16]:

$$\frac{\partial \rho(q, q', t)}{\partial t} = -\frac{\gamma}{8}(q - q')^2 \rho(q, q', t), \quad (4)$$

which means that the off-diagonal elements of the density matrix decay exponentially with a rate given by γ times the square of the distances between the corresponding positions. We should keep this decay rate modest compared to the rate of the Schrödinger evolution due to the Hamiltonian \hat{H} of the monitored particle. Low values of the strength γ may, however, result in low efficiency of position monitoring and slow convergence of our method of wave function estimation, cf section 4. The above constraint on $\sigma^2 \tau$ can in general be matched with further ones—see the [appendix](#)—that ensure the applicability of the continuum limit and its analytic equations.

3. Monitoring the wave function

While it seems plausible that after a sufficiently long time t the sequence of unsharp position measurements provides enough data to estimate $|\psi_t(q)|^2$, it may come as a surprise that position measurements enable a faithful monitoring of the full wave function $\psi_t(q)$ as well. The reason for this is as follows. Measuring the position \hat{q} at times $t = \tau, 2\tau, \dots$ on a system with evolving Schrödinger wave function ψ_t is equivalent to consecutive measurements of the Heisenberg observables $\hat{q}_t = \exp(it\hat{H})\hat{q}\exp(-it\hat{H})$ on a system with static wave function ψ_0 . The set of Heisenberg coordinates $\{\hat{q}_t\}$ will exhaust a sufficiently large space of incompatible observables so that their measurements will lead to a faithful determination of ψ_0 and—in this way—to our faithful determination of ψ_t for long enough times t . In the degenerate case $\hat{H} = 0$, monitoring turns out to be trivial: for long enough times, a large number t/τ of unsharp position measurements of resolution σ is equivalent to a single sharp measurement of resolution $\sigma/\sqrt{t/\tau}$; position monitoring thus yields just preparation of a static sharply localized wave function—an approximate ‘eigenstate’ of \hat{q} .

Our monitoring of the wave function means a real-time estimation of it, where the quality of monitoring depends on the fidelity of the estimation. We start from a certain initial estimate ψ_0^e and simulate its evolution according to the self-dynamics of the particle, which is assumed to be known, until time $t = \tau$. Immediately after we have learned the first position \bar{q}_τ from the first measurement on the particle, we update the estimate according to the same rule (1) as the actual wave function of the particle and renormalize it:

$$\psi_\tau^e(q) \longrightarrow \text{normalization} \times \sqrt{G_\sigma(q - \bar{q}_\tau)} \psi_\tau^e(q). \quad (5)$$

This update resembles the Bayes principle of non-parametric statistical estimation. We repeat this procedure for $t = 2\tau, 3\tau, \dots$ expecting that the estimated ψ_t^e and the observed wave function ψ_t will converge! A rigorous proof of convergence is missing. In the continuum limit, nonetheless, it was conjectured that convergence occurs if the common eigenspace of

all Heisenberg operators \hat{q}_t is empty or one-dimensional [20]. As an illustration, consider the case of independent dynamics in the two coordinates \hat{x}, \hat{y} , where only the coordinate \hat{x} is monitored and the above condition is thus not met; the estimate will in general not converge to the true wave function. However, measurement of one of the coordinates—say \hat{x} —yields the desired convergence according to the conjecture, for example, if the unitary dynamics rotates the Heisenberg operator \hat{x}_t in the plane spanned by both coordinates. Rather than pursuing the rigorous theoretical conditions of convergence cf [21], we turned to numerical tests of continuous measurements that have definitely confirmed our method.

4. Numerical simulations

We simulated the evolution of a single hydrogen atom subjected to continuous measurements at several potentials. However, the conclusions of our discussion are not restricted to hydrogen atoms; similar results can be expected for atoms with higher masses in appropriately scaled potentials.

The coupled evolutions of the wave function, measurement readout and the estimated wave function were simulated numerically by discretizing the corresponding stochastic differential equations (cf the [appendix](#)). For this purpose, we employed a numerical algorithm of Kloeden and Platen, which is accurate up to second order in the time step of the discretization [18, 22].

In order to study the relation between the evolution of the wave function of the particle, on the one hand, and the evolution of its estimate, on the other hand, we first confine ourselves to a one-dimensional spatial motion. In this case, the graphical representation is the simplest and thus gives a clear picture of the convergence between real and estimated wave functions. As an example we consider a hydrogen atom situated in a quartic double well potential with a shape as depicted in figure 1.

We assume a continuous measurement of the position of the hydrogen atom with strength $\gamma = 9.9856 (\mu\text{m})^2 \text{s}^{-1}$. In order to get an impression of the dimensions of the measurement, let us invoke equation (3) to note that this value of γ may correspond, e.g., to single Gaussian measurements with a spatial resolution of $\sigma = 1.4 \text{ nm}$ repeated at time periods $\tau = 50 \text{ ns}$. The spatial resolution of the single weak measurements [23] is thus 140 times poorer than the width $\sigma = 10 \mu\text{m}$ of the initial Gaussian wave function of the atom. In figure 1, we have depicted snapshots recorded at different times of the spatial probability density $|\psi(x)|^2$ of the H atom (blue solid line) and the squared modulus $|\psi^e(x)|^2$ of the estimated wave function (red dashed line). Initially, both probability densities assume the form of Gaussians that differ in width and location within the double-well potential. The sequence of pictures demonstrates the convergence of the densities in the course of a continuous measurement.

The real probability density $|\psi(x)|^2$ of the H atom, which possesses initially a slightly higher mean energy than the middle peak of the potential, oscillates back and forth between the sides of the potential. The oscillatory motion of the centre of $|\psi(x)|^2$ would also be expected qualitatively without measurements—as well as from a classical particle of the same mass moving in the double well. However, the real probability density does not spread as it would without measurements. This localization effect caused by the continuous unsharp position measurement adapts the motion of the H atom to that of a classical particle that is perfectly localized at each instance. This illustrates the influence of the measurements and points to a particular kind of control of the wave function that can be exercised by means of unsharp position measurements. A smaller measurement strength would lead to less disturbance of

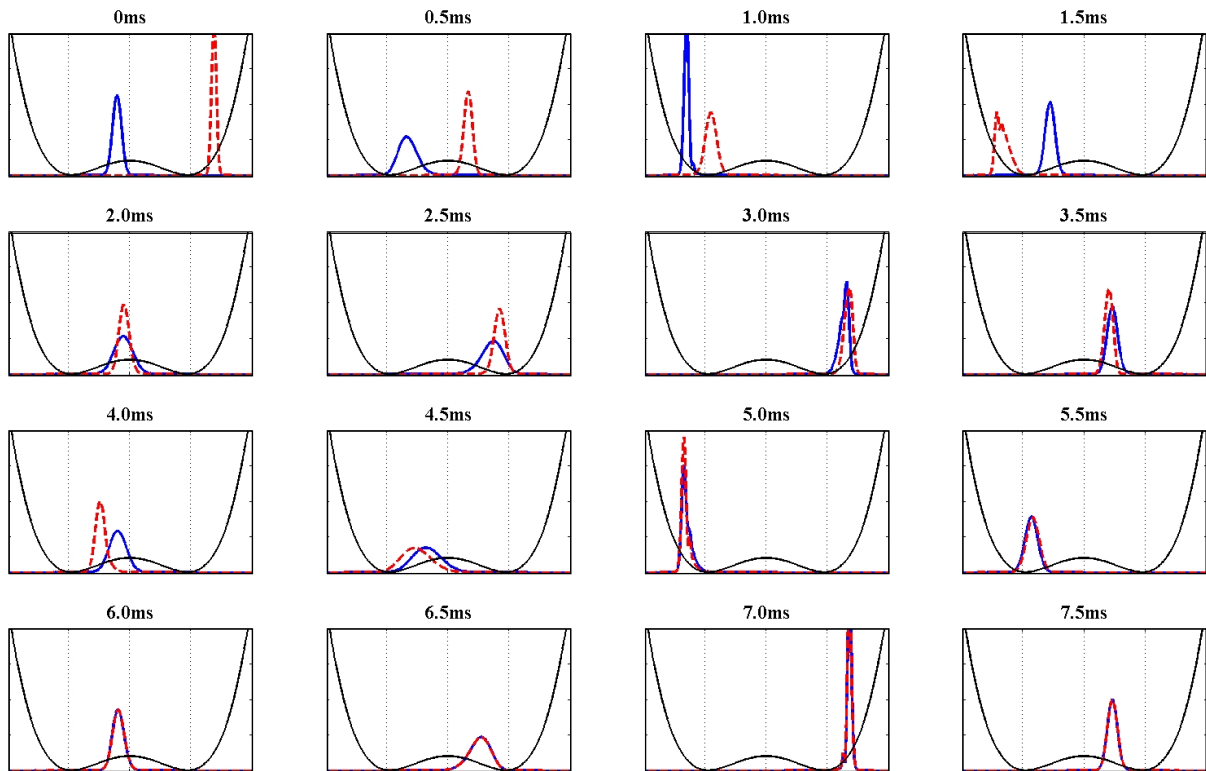


Figure 1. Motion in a double-well potential. The frames show a time sequence of the real probability density of atomic position $|\psi|^2$ (blue solid line) and the estimated probability density $|\psi^e|^2$ (red dashed line). The solid black line represents the double-well potential as a function of position. Its minima are $189 \mu\text{m}$ apart and the height of the central maximum is given by $1 \times 10^{-13} \text{ eV}$.

the unitary motion in the potential, but also to lower speed of convergence between real and estimated probability densities.

The estimated probability density $|\psi^e(x)|^2$, which is centred initially on the right-hand side of the potential, follows the real wave function until after approximately one oscillation period, the corresponding probability densities coincide and evolve identically thereafter. But not only the probabilities to find the atom at a certain position converge, in fact the complete wave function $\psi(x)$ and its estimate $\psi^e(x)$ coincide after a sufficiently long period! It can be proved analytically that the estimation fidelity $F = |\langle \psi | \psi^e \rangle|$, which measures the overlap between the wave functions ψ and ψ^e , when averaged over many realizations of the continuous measurement, increases with time and converges to 1 [20]. Numerical simulations for the double-well potential show that in a typical realization with initial values as described above and measurement strength $\gamma = 9.9856 (\mu\text{m})^2 \text{ s}^{-1}$ the fidelity amounts to more than 95% after 1.5 oscillation periods.

Figure 2 shows the evolution of estimation fidelity for a continuously measured H atom moving in a plane under the influence of a Mexican-hat potential. The latter is a rotationally symmetric version of the double well in two spatial dimensions. For the sake of simplicity, we assume that both position coordinates are simultaneously and independently measured with the same strength γ . Such a continuous measurement of both the coordinates typically yields

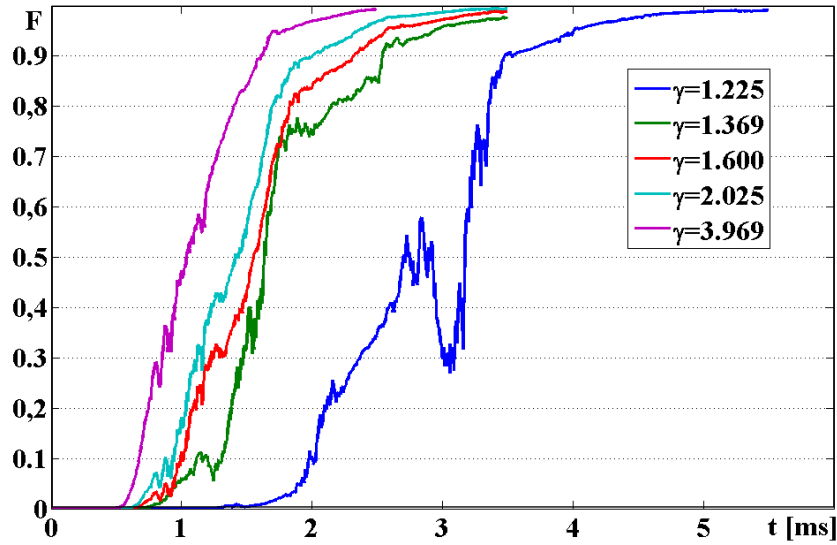


Figure 2. Estimation fidelity for the Mexican-hat potential. The fidelity of estimation F is plotted as a function of the duration of continuous measurement of an H atom moving in a Mexican-hat potential for different values of measurement strength γ in units of $10 (\mu\text{m})^2 \text{s}^{-1}$. The height of the Mexican hat's central peak situated at the origin of the reference frame is given by $1.07 \times 10^{-12} \text{ eV}$, its minima lie on a concentric circle with a radius of $40 \mu\text{m}$ around the origin. The wave function $\psi(x)$ and its estimate $\psi^e(x)$ are initially Gaussians centred at $(-55, -14.8 \mu\text{m})$ and $(-103.6, -103.6 \mu\text{m})$ with widths of $10 \mu\text{m}$ as well as $5 \mu\text{m}$, respectively. The plots demonstrate that perfect fidelity is reached eventually for all considered measurement strengths. However, the convergence time decreases with increasing γ .

evolutions of the estimation fidelities, which are shown in figure 2 for several values of the measurement strength γ . In all depicted cases, the fidelity comes very close to 1 within a period of 5 ms, i.e. estimated and real wave functions then coincide. Thereafter the dynamics of the wave function including the influence of the measurement can thus be monitored with perfect fidelity.

One might doubt that our monitoring remains efficient for heavily complex wave functions like those developing in classically chaotic systems. Instead of the integrable Mexican-hat potential, this time we study the chaotic Hénon–Heiles potential, which depends on the radius r as well as on the azimuth ϕ :

$$V(x, y) = A [r^4 + ar^2 + br^3 \cos(3\phi)] . \quad (6)$$

For this potential, we simulated continuous position measurement and monitoring with the following results. The saturation of fidelity is reassuring: the estimate converges to the real wave function (figure 4), which is found at a slightly longer time scale than in the integrable Mexican-hat potential, whereas the wave functions show an apparently irregular complex structure. Figure 3 shows the estimated and real wave functions with an average overlap (i.e. a fidelity) of 91.58%. Indicating already an accurate overall estimation of the real wave function, this value still includes in small areas of the potential differences of the corresponding probability densities

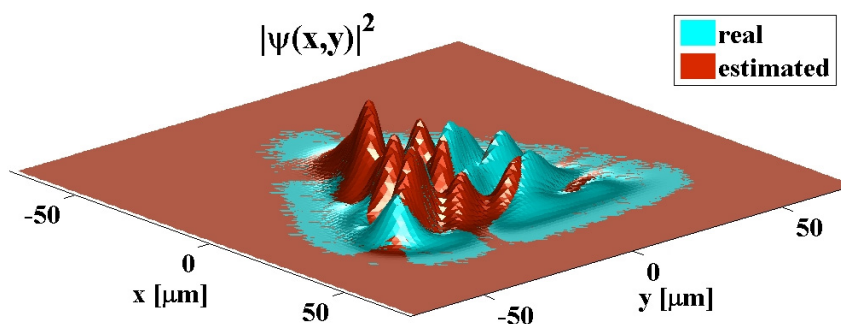


Figure 3. Monitoring of complex wave functions. The real (blue) and estimated (red) spatial probability densities $|\psi|^2$ and $|\psi^e|^2$, whichever assumes a greater value, are depicted in the Hénon–Heiles potential after time 3.15 ms, at fidelity 0.9158, for the same initial states as in figure 4.

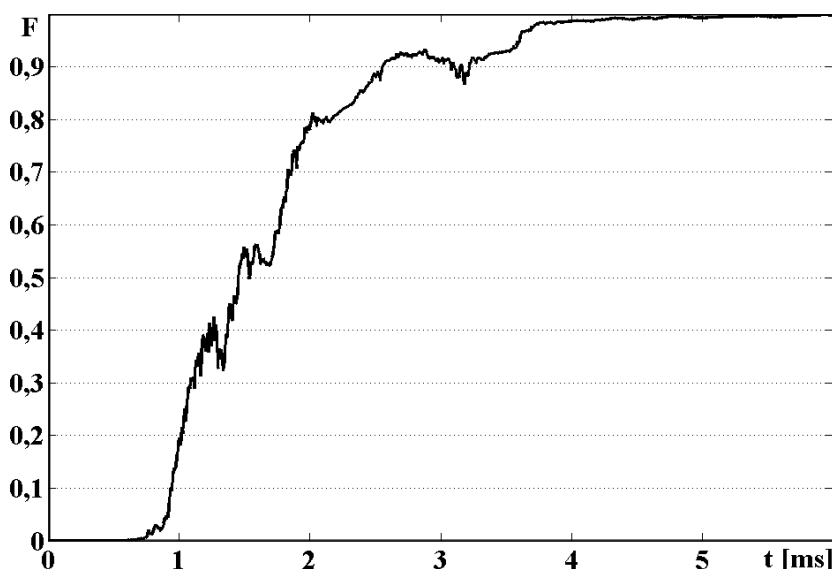


Figure 4. Convergence for the Hénon–Heiles potential. The fidelity of estimation F is plotted as a function of the duration of the continuous measurement at strength $\gamma = 12.351 (\mu\text{m})^2 \text{s}^{-1}$ of a H atom in the non-integrable Hénon–Heiles potential (6) with parameters $A = 5.44 \times 10^{-17} \text{eV} (\mu\text{m})^{-4}$, $a = 13.09 \mu\text{m}^2$ and $b = 36.18 \mu\text{m}$. The wave function $\psi(x)$ and its estimate $\psi^e(x)$ are initially Gaussians centred at $(-14.8, -29.6 \mu\text{m})$ and $(-29.6, -29.6 \mu\text{m})$, both with widths of $10 \mu\text{m}$, respectively. We find that the fidelity converges to 1 and therefore our estimate becomes a good approximation of the real wave function.

up to 35% of their highest peak. In particular, figure 3 indicates that faithful monitoring is not only possible when the shape of the wave function of the particle is close to a Gaussian, but also for rather complex shapes.

Monitoring, i.e. continuous unsharp observation, has a specific capacity. It is its robustness against external unexpected perturbations. To demonstrate such a robustness, we assumed that close to saturation of the estimation fidelity, as in figure 3, our atom in the

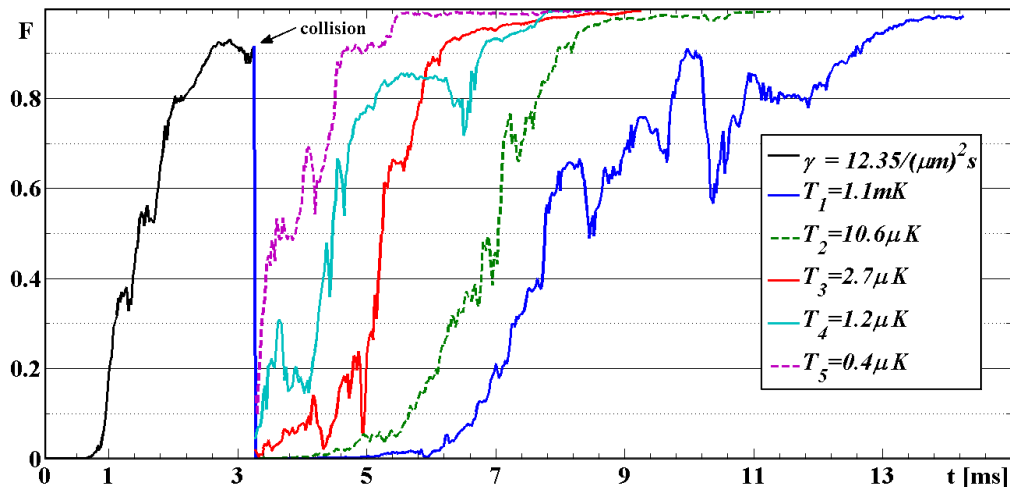


Figure 5. Robustness of the estimation scheme. At $t = 3.15$ ms and fidelity 0.9158, exactly when the snapshot of figure 3 was taken, the H atom is hit by another thermal H atom, which causes an immediate drop in fidelity. We supposed a single momentum transfer $p_x = \sqrt{mk_B T}$ in the x -direction only, at different temperatures. The fidelity recovers and converges to 1 after some time, which depends on the temperature, i.e. on the strength of the momentum kick.

Hénon–Heiles potential is suddenly perturbed, e.g., by a collision with an environmental particle (here another hydrogen atom). For simplicity, we assume a momentum kick p_x along the x -direction, which implies a multiplication of the real wave function by the complex function $\exp(ip_x x/\hbar)$; hence the estimated wave function has to start a new cycle of convergence. We map the momentum kick p_x to a temperature by $k_B T = p_x^2/m$ as if it had a thermal origin, just to give a hint of its strength. Numeric results (figure 5) show that the estimation fidelity recovers against these momentum perturbations (cf supplementary video, available from stacks.iop.org/NJP/12/043038/mmedia). In reality, repeated random perturbations might prevent perfect monitoring and fidelity will saturate at less than 1. Although this case is beyond the scope of our present work, its study will be of immediate interest since real systems are subject to various noises that are not measured at all. The monitoring theory at non-optimum efficiency has been outlined earlier [20].

5. Discussion

We simulated numerically continuous position measurements carried out on a single quantum particle in one- and two-dimensional potentials. In order to monitor the evolution of an initially unknown state of the particle in a known potential, we estimated its wave function and updated the estimate continuously employing the measurement results.

Our simulations show that for all the considered potentials, the overlap between estimated and real wave functions comes close to 1 after a finite period of measurement—guaranteeing thereafter precise knowledge of the particle’s state and real-time monitoring of its further evolution with high fidelity. The power of our method is indicated by the ability to monitor even the motion of a particle in a classically chaotic potential subjected to continuous position measurement.

We have thus demonstrated that monitoring the complete state of a quantum system with infinite-dimensional state space is feasible by continuously measuring a single observable on a single copy of the system. Moreover, the simulations indicate that our monitoring method is robust against sudden external perturbations such as occasional random momentum kicks. How much and what kinds of external noise this monitoring scheme tolerates is important for its applicability in control and error correction tasks, and might be the object of future research. As an example of a control task, we mention the cooling of a mechanical oscillator by position monitoring augmented with feedback in the form of counter momentum transfer.

Acknowledgments

We acknowledge the support of the Bilateral Hungarian–South African R&D Collaboration Project, Hungarian OTKA grants 49384 and 75129 and South African NRF Focus Area grant 65579. We thank J Audretsch and A Scherer for discussions. In particular, we are grateful to Ronnie Kosloff for his suggestion that we also monitor chaotic dynamics. This work is partly based on research supported by the South African Research Chairs Initiative of the Department of Science and Technology and National Research Foundation.

Appendix. The Itô method

The discrete sequence of unsharp measurements (1, 2) and wave function updates (5) possess their continuum limit [24] if we take $\tau \rightarrow 0$ and $\sigma^2 \rightarrow \infty$ at $1/\gamma = \tau\sigma^2 = \text{const}$. In this ‘continuum limit’, both the true wave function $\psi_t(q)$ and the estimated wave function $\psi_t(q)$ become continuous stochastic processes such that they are tractable by two stochastic differential equations, respectively. The position measurement outcomes \bar{q}_t do not yield a continuous stochastic process themselves. It is their time integral Q_t , specified below, that becomes a continuous stochastic process.

Let us consider the discrete increment of the true wave function during the period τ , cf equation (1). In Dirac formalism, we obtain

$$\Delta|\psi\rangle = \exp(-i\tau\hat{H}) \frac{1}{p(\bar{q})} \sqrt{G_\sigma(\hat{q} - \bar{q})} |\psi\rangle - |\psi\rangle. \quad (\text{A.1})$$

For simplicity, we omit notations of time dependence t . The symbol $\langle\hat{q}\rangle$ stands for $\langle\psi_t|\hat{q}|\psi_t\rangle$. In the continuum limit, equation (A.1) transforms into the following Itô-stochastic differential equation [3]:

$$d|\psi\rangle = \left(-i\hat{H} - \frac{\gamma}{8}(\hat{q} - \langle\hat{q}\rangle)^2\right) dt|\psi\rangle + \frac{\sqrt{\gamma}}{2}(\hat{q} - \langle\hat{q}\rangle)(dQ - \langle\hat{q}\rangle dt)|\psi\rangle. \quad (\text{A.2})$$

The equation of the discrete increment $\Delta|\psi^e\rangle$ of the estimate (slight change) assumes the same form as equation (A.1) of $\Delta|\psi\rangle$ but the normalization factor differs from $1/p(\bar{q})$, cf equation (5). Yet, it yields the same Itô stochastic differential equation as the equation above. The estimated state $|\psi_t^e\rangle$ must be evolved according to the same nonlinear differential equation (A.2) that describes the evolution of the monitored particle’s state $|\psi_t\rangle$. These two equations are coupled via the stochastic process Q , whose discrete increment is defined by $\Delta Q = \bar{q}\tau$; in the continuum limit this means formally $Q_t = \int_0^t \bar{q}_s ds$, where \bar{q}_s is the measured position at time s . In reality, the random process Q_t is obtained from the measured data $\{\bar{q}_t\}$. If the measurement

is just simulated, like in our work, then in the continuum limit ΔQ transforms into the Itô differential dQ whose random evolution can be generated by the standard Wiener process W via $dQ = \langle \hat{q} \rangle dt + \gamma^{-1/2} dW$. Of course, Q_t breaks the symmetry between the stochastic processes ψ_t and ψ_t^e because dQ/dt fluctuates around $\langle \psi_t | \hat{q} | \psi_t \rangle$ and not around $\langle \psi_t^e | \hat{q} | \psi_t^e \rangle$.

The stochastic differential equation (A.2)—combined with the same one for $|\psi^e\rangle$ —is a suitable approximation of our discrete model (see above) under two conditions. (i) A single measurement does not resolve any particular structure of the wave function, i.e. $\sigma \gg \sigma_\psi$, where σ_ψ is the width of the spatial area on which ψ is not negligibly small. Thus σ_ψ can, e.g., be of the order of magnitude of the available width of the confining potential. (ii) The length of the time period τ between two consecutive measurements is small compared to the timescale of self-dynamics generated by the Hamiltonian \hat{H} . Then the discrete model of position monitoring and wave function estimation becomes tractable by the time-continuous equation (A.2) depending on the single parameter $1/\gamma = \tau\sigma^2$, cf equation (3).

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