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Bayesian approach to inverse quantum statistics: Reconstruction of potentials in the Feynman path integral representation of quantum theory

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Abstract. The Feynman path integral representation of quantum theory is used in a non–parametric Bayesian approach to determine quantum potentials from measurements on a canonical ensemble. This representation allows to study explicitly the classical and semiclassical limits and provides a unified description in terms of functional integrals: the Feynman path integral for the statistical operator and its derivative with respect to the potential, and the integration over the space of potentials for calculating the predictive density. The latter is treated in maximum a posteriori approximation, and various approximation schemes for the former are developed and discussed. A simple numerical example shows the applicability of the method.

PACS. 02.50.Tt Inference methods – 31.15.Kb Path-integral methods – 05.30.-d Quantum statistical mechanics

1 Introduction

The solution of the quantum many–body problem requires both techniques for solving the Schrödinger equation and knowledge of the underlying forces, often to be deduced from observational data. In the field of nuclear physics, forces are extracted from scattering data and ground state properties of the two–nucleon system, since no practicable basic theory of nuclear forces exists up to date. Given a data–based phenomenological nucleon–nucleon potential, one can, in principle, construct the related potential between two colliding nuclei. However, this is a formidable task which has been attacked only for a few simple cases in an approximate way, and a direct calculation of the nucleus–nucleus potential from observational data is highly desirable for practical applications like, e.g., in nuclear astrophysics. In solid state physics the basic force is known to be the Coulomb force, however, for a straight problem like the motion of a single electron under the influence of a crystal surface, one would prefer to deduce the respective potential directly from observational data rather than going through the full many–body problem of electrons and nuclei of the crystal.

The reconstruction of such two–body forces or single–particle potentials from experimental data constitutes a typical inverse problem of quantum theory. Such problems are notoriously ill–posed in the sense of Hadamard [1] and require additional a priori information to obtain a unique, stable solution. Well–known examples are inverse scattering theory [2] and inverse spectral theory [3]. They describe the kind of data which are necessary, in addition to a given spectrum, to identify the potential uniquely. For example, such data can be a second spectrum for different boundary conditions, knowledge of the potential on a half–interval or the phase shifts as a function of energy. However, neither a complete spectrum nor specific values of the potential or phase shifts at all energies can be inferred by a finite number of measurements. Hence any practical algorithm for extracting two–body forces or single–particle potentials from experimental data must rely on additional a priori assumptions like symmetries, smoothness, or asymptotic behaviour. If the available data refer to a system at finite temperature $T \neq 0$, one is led to the inverse problem of quantum statistics. In such a case, non–parametric Bayesian statistics [4] is especially well suited to include both observational data and a priori information in a flexible way.

In a series of papers [5], the Bayesian approach to inverse quantum statistics has been applied to reconstruct potentials (or two–body interactions) from particle–position measurements on a canonical ensemble. A priori information was imposed through approximate symmetries (translational, periodic) or smoothness of the potential or by fixing the mean energy of the system. The likelihood model of quantum statistics (defining the probability for finding the particle at some position x for a system with potential V at temperature T) was treated in energy representation.

In the present paper we apply the Feynman path integral representation of quantum mechanics [6] to calculate

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matrix elements of the statistical operator ρ and related quantities in coordinate space. This representation is of interest in the context of inverse problems in Bayesian statistics for two reasons: First, it allows to study the transition to the semiclassical and classical limits, relevant for example to atomic force microscopy [7] so far treated on the level of classical mechanics. However, scales may soon be reached where the inclusion of quantum effects will be mandatory. Second, one obtains a unified description of Bayesian statistics in terms of functional integrals. These are on one side the Feynman path integrals, needed in the likelihood model, and on the other side the functional integral over the space of potential functions V when calculating the predictive density as integral over the product of likelihood and posterior for all possible potentials.

Our paper is organized as follows: An introduction to Bayesian statistics is presented in Section 2, showing how Bayes' theorem about the decomposition of joint probabilities can be used for the inverse problem of quantum statistics. A general expression is given for the likelihood of a quantum system with given potential V for a canonical ensemble, and the prior density is chosen as Gaussian process to implement a bias towards smoothness and/or periodicity of the potential V. This potential can be calculated from a non–linear differential equation which results from the maximum posterior approximation for the predictive density. In Section 3 we develop exact expressions, in terms of path integrals, for the likelihood and its variation with respect to the potential. Two approximation schemes for solving the inverse problem of quantum statistics in path integral representation are proposed.

In the first variant, the path integrals in the likelihood are treated in stationary phase approximation (Sect. 4). Variation of the resulting, approximate likelihood with respect to the potential then defines the maximum posterior approximation on the semiclassical level ("variation after approximation"). Quantum fluctuations around the classical paths of Section 4 are determined in Section 5, and the classical limit is studied.

In the second variant, we invert the order of the above operations ("variation before approximation"): We start from the exact stationarity equations of the maximum posterior approximation, expressed by the path integrals and their derivatives, which are then treated in stationary phase approximation in Section 6, with details given in the appendix.

A simple numerical example is added in Section 7 to demonstrate that the path integral formalism can actually be used for problems of inverse quantum statistics. Our conclusion (Sect. 8) discusses in particular the relations between the various approximation schemes developed in this paper, and their numerical implications.

2 Bayesian approach to inverse quantum statistics

The aim of this paper is to determine the dynamical laws of quantum systems from measurements on a canonical ensemble. The method used is non-parametric Bayesian inference combined with the path integral representation of quantum theory which allows to study the transition to the classical limit. To be specific, we aim at reconstructing the potential V of the system from measurements of the position coordinate $\hat{x}$ of the particle for a canonical ensemble at temperature $1 / \beta$.

The general Bayesian approach, tailored to the above problem, is based on two probability densities:

1. a likelihood $p\,(x|O,\, V)$ for the probability of outcome x, given a device for measuring observable O and given potential V, not directly observable, and
2. a prior density $p\,(V)$ defined on the space $\mathcal{V}$ of possible potentials V.

This prior gives the probability for V before data have been collected. Hence it has to comprise all a priori information available for the potential, like symmetries, smoothness, or asymptotic behaviour. The need for a prior model, complementing the likelihood model, is characteristic for empirical learning problems which try to deduce a general law from observational data.

These ingredients, likelihood and prior, are combined in Bayes theorem to define the posterior of V for given data D through

$$p\,(V|D) \,=\, \frac{p\,(x_T|O_T,\, V)\,p\,(V)}{p\,(x_T|O_T)}\ . \tag{2.1}$$

Equation (2.1) is a direct consequence of the decomposition of the joint probability $p\,(A,\, B)$ for two events A, B into conditional probabilities $p\,(A|B)$ and $p\,(B|A)$, respectively. Observational data D are assumed to consist of N pairs,

$$D = \{(x_i,\, O_i)|1 \,\leq\, i \,\leq\, N\}\ , \tag{2.2}$$

where x_T, O_T denote formal vectors with components x_i, O_i. Such data are also called training data, hence the label $_T$. For independent data the likelihood factorizes as

$$p\,(x_T|O_T,\, V) \,=\, \prod_i\, p\,(x_i|O_i,\, V)\ , \tag{2.3}$$

where a chosen observable O_i may be measured repeatedly to give values x_i, equal or different among each other. The denominator in (2.1) can be viewed as normalization factor and can be calculated from likelihood and prior by integration over V,

$$p\,(x_T|O_T) \,=\, \int DV\ p\,(x_T|O_T,\, V)\,p\,(V)\ . \tag{2.4}$$

The V-integral in equation (2.4) stands for an integral over parameters, if we choose a parametrized space $\mathcal{V}$ of potentials, or for a functional integral over an infinite function space.

To predict the results of future measurements on the basis of a data set D, one calculates according to the rules of probability theory the predictive density

$$p\,(x|O,\, D) \,=\, \int DV\ p\,(x|O,\, V)\,p\,(V|D) \tag{2.5}$$

which is the probability of finding value x when measuring observable O under the condition that data D are given. Here we have assumed that the probability of x is completely determined by giving potential V and observable O, and does not depend on training data D, $p\,(x|O,\,V,\,D)\,=\,p\,(x|O,\,V)$, and that the probability for potential V given the training data D does not depend on observable O selected in the future, $p\,(V|O,\,D)\,=\,p\,(V|D)$.

The integral (2.5) is high-dimensional in general and difficult to calculate in practice. Two approximations are common in Bayesian statistics: The first one is an evaluation of the integral by Monte Carlo technique. The second one, which we will pursue in this paper, is the so called maximum a posteriori approximation. Assuming the posterior to be sufficiently peaked around its maximum at potential V^*, the integral (2.5) is approximated by

$$p\,(x|O,\,D)\,\approx\,p\,(x|O,\,V^*) \tag{2.6}$$

where

$$\begin{aligned} V^* &= \mathrm{argmax}_{V\,\in\,\mathcal{V}}\,p\,(V|D) \\ &= \mathrm{argmax}_{V\,\in\,\mathcal{V}}\,p\,(x_T|O_T,\,V)\,p\,(V) \end{aligned} \tag{2.7}$$

according to equation (2.1) with the denominator independent of V. Maximizing the posterior $p\,(V|D)$ with respect to $V\,\in\,\mathcal{V}$ leads to solving the stationarity equations

$$\delta_V\,p\,(V|D)\,=\,0\,=\,\delta_V\,(p\,(x_T|O_T,\,V)\,p\,(V)) \tag{2.8}$$

where δ_V denotes the functional derivative $\delta\,/\,\delta\,V$. Equivalent to (2.8) and technically often more convenient is the condition for the log-posterior

$$\delta_V\,\ln\,p\,(V|D)\,=\,0\,=\,\delta_V\,\ln\,p\,(x_T|O_T,\,V)\,+\,\delta_V\,\ln\,p\,(V) \tag{2.9}$$

which minimizes the energy $E\,(V|D)\,=\,-\ln\,p\,(V|D)$ and will be used in the following.

A convenient choice for prior $p\,(V)$ is a Gaussian process,

$$p\,(V)\,\sim\,\exp\,\left\{-\frac{\gamma}{2}\,\langle V\,-\,V_0|K|V\,-\,V_0\rangle\right\}\,=\,\mathrm{e}^{-\frac{\gamma}{2}\,\Gamma\,[v]} \tag{2.10}$$

where

$$\begin{aligned} \Gamma\,[v] &= \langle V-V_0|K|V-V_0\rangle \\ &= \int dx\,dx'\;[v\,(x)-v_0\,(x)]\,K\,(x,\,x')\,[v\,(x')-v_0\,(x')], \end{aligned} \tag{2.11}$$

assuming a local potential $V\,(x,\,x')\,=\,v\,(x)\,\delta\,(x\,-\,x')$. The mean V_0 represents a reference potential or template for V, and the real-symmetric, positive (semi-)definite covariance operator $(\gamma\,K)^{-1}$ acts on the potential, measuring the distance between V and V_0. The hyperparameter γ is used to balance the prior against the likelihood term and is often treated in maximum a posteriori approximation or determined by cross–validation techniques. A bias towards smooth solutions $v\,(x)$ of the stationarity equation (2.9) can be implemented by $K\,=\,-d^2\,/\,dx^2$ choosing $v_0\,(x)\,\equiv\,0$. While a typical potential generated by a Wiener process is only continuous, solutions $v(x)$ of the stationarity equation (2.9) are differentiable, unless the functional derivative of the likelihood has a δ-spike at some location x. To enhance smoothness in the sense of differentiability of solutions of equation (2.9) one may include higher powers of Δ, for example, through the choice $K=\sum_{k=1}^{p}\,\frac{(-1)^k}{k!}\,\left(\frac{\sigma_0^2\,\Delta}{2}\right)^k$ [4,8]. If some approximate symmetry of $v\,(x)$ is expected, like for a surface of a crystal deviating from exact periodicity due to point defects, one may implement a non-zero periodic reference potential $v_0\,(x)$ in equation (2.11).

The likelihood for our problem follows from the axioms of quantum theory: The probability to find value x when measuring observable O for a quantum system in a state described by a statistical operator $\rho\,=\,\rho\,(V)$ is given by

$$p\,(x|O,\,V)\,=\,\mathrm{Tr}\,\{P_O\,(x)\,\rho\,(V)\} \tag{2.12}$$

where $P_O\,(x)\,=\,\Sigma_\xi\,|x,\,\xi\rangle\,\langle x,\,\xi|$ projects on the space spanned by the orthonormalized eigenstates $|x,\,\xi\rangle$ of operator O with eigenvalue x, and the label ξ distinguishes degenerate eigenstates with respect to O. If the system is not prepared in an eigenstate of observable O, a quantum mechanical measurement will change the state of the system, i. e., will change ρ. Hence to perform repeated measurements under same ρ requires the restoration of ρ before each measurement. For canonical ensembles at given temperature,

$$\rho=\frac{\exp(-\beta\,H)}{\mathrm{Tr}\exp(-\beta\,H)} \tag{2.13}$$

with Hamiltonian $H\,=\,T\,+\,V$ and temperature $1\,/\,\beta$, this means to wait between two consecutive observations until the system is thermalized again. Choosing the particle position operator $\hat{x}$ as observable O, the probability for value x_i is

$$p\,(x_i|\hat{x},\,v)=Z^{-1}\,\mathrm{Tr}\{|x_i\rangle\,\langle x_i|\,\exp\,(-\beta\,H)\}=\frac{\langle x_i|\mathrm{e}^{-\beta\,H}|x_i\rangle}{Z} \tag{2.14}$$

with partition function

$$Z\,=\mathrm{Tr}\exp\,(-\beta\,H)\,=\,\int dx\;\langle x|\exp\,(-\beta\,H)|x\rangle \tag{2.15}$$

where we have dropped the label ξ to simplify notation. For N repeated measurements of $\hat{x}$ with results x_i, $i\,=\,1,\,...\,N$, one has under the above assumptions of independent measurements

$$p\,(x_T|O_T,\,V)=\prod_i\,p\,(x_i|\hat{x},\,v)=\prod_i\,\left[\langle x_i|\mathrm{e}^{-\beta\,H}|x_i\rangle\,Z^{-1}\right]. \tag{2.16}$$

Combining equations (2.10), (2.11) and (2.16) leads to the posterior

$$p\,(V|D)\,\sim\,\frac{1}{Z^N}\,\left(\prod_i\,\langle x_i|\mathrm{e}^{-\beta\,H}|x_i\rangle\right)\,\exp\,\left(-\frac{\gamma}{2}\,\Gamma\,[v]\right)= \exp\,(-E\,(V|D)) \tag{2.17}$$

with energy functional

$$E\,(V|D)\;=\;-\sum_i\,\ln\,\langle x_i|\mathrm{e}^{-\beta\,H}|x_i\rangle\;+\;N\,\ln\,Z\;+\;\frac{\gamma}{2}\,\Gamma\,[v]\;, \tag{2.18}$$

functional $\Gamma\,[v]$ defined in equation (2.11). The corresponding stationarity equations (2.9) in explicit form read

$$-\sum_{i\,=\,1}^{N}\,\frac{\frac{\delta}{\delta\,v\,(x)}\,\langle x_i|\mathrm{e}^{-\beta\,H}|x_i\rangle}{\langle x_i|\mathrm{e}^{-\beta\,H}|x_i\rangle}\,+\,\frac{N}{Z}\,\frac{\delta\,Z}{\delta\,v\,(x)}\,+\,\frac{\gamma}{2}\,\frac{\delta\,\Gamma}{\delta\,v\,(x)}\;=\;0\;, \tag{2.19}$$

with

$$\frac{1}{2}\frac{\delta\,\Gamma}{\delta\,v\,(x)}=\int dx'\,K(x,x')\,(v\,(x')\;-\;v_0\,(x'))\;. \tag{2.20}$$

To extract the unknown potential $v(x)$ from the above non–linear variational equations one may use the algorithm

$$v^{(r+1)}=v^{(r)}-\eta A^{-1}\frac{\delta}{\delta v}\left\{\ln p(v^{(r)})+\sum_i\ln p(x_i|\hat{x},v^{(r)})\right\}, \tag{2.21}$$

to be iterated till convergence is obtained. Step length $\eta>0$ can be optimized during iteration. One may choose any suitable positive definite operator A. For example, taking $A=1$ the algortihm is known as gradient descent, for the prior (2.20) $A=K$ is typically also a good choice.

In a series of papers [5], equations (2.19) have been studied successfully in energy representation for a variety of choices for prior $p\,(V)$. This requires solving the Schrödinger equation $H\,|\phi_\alpha\rangle\;=\;E_\alpha\,|\phi_\alpha\rangle$, $\langle\phi_\alpha|\phi_\beta\rangle\;=\;\delta_{\alpha\beta}$, which allows to calculate the functional derivatives $\delta_v\,E_\alpha$ and $\delta_v\,\phi_\alpha$ needed in equations (2.19). In the following sections we shall apply the path integral formulation of quantum mechanics in order to study the semiclassical as well as classical regimes.

3 Likelihood and posterior in path integral representation

To begin with we will give exact path integral representations for the statistical operator, for the partition function, and their derivatives with respect to the potential. These quantities constitute likelihood (2.16), posterior (2.17), and the stationarity equations (2.19) defining the maximum of the posterior.

The matrix elements appearing in the likelihood (2.16) can be written as path integrals [6]

$$\langle x_i|\mathrm{e}^{-\beta\,H}|x_i\rangle\;=\;\int\limits_{q\,(0)\,=\,x_i}^{q\,(\beta\,\hbar)\,=\,x_i}Dq\,(\tau)\,\exp\left\{-\frac{1}{\hbar}\int\limits_0^{\beta\,\hbar}d\tau\,\left(\frac{m}{2}\,(dq\,/\,d\tau)^2+v\,(q)\right)\right\}. \tag{3.1}$$

They are related to those of the time development operator of quantum mechanics by Wick rotation in the complex time plane. The corresponding variable transformation

$$t\;=\;-i\,\tau \tag{3.2}$$

replaces real time t by imaginary time τ and velocity $dq\,/\,dt$ by

$$\frac{dq}{d\tau}\;=\;-i\frac{dq}{dt}\,, \tag{3.3}$$

inducing a change of sign in the kinetic energy term.

Representation (3.1) is understood as abbreviation of an infinite dimensional integral when dividing the interval $[0,\,\beta\,\hbar]$ into equidistant segments of length $\varepsilon\;=\;\beta\,\hbar\,/\,M$, coding the path $q\,(\tau)$ at discrete points $\tau_k\;=\;\varepsilon\,k$ by $q_k\;=\;q\,(\tau_k)$ and taking the limit $M\;\to\;\infty$

$$\begin{aligned}\langle x_i|\mathrm{e}^{-\beta\,H}|x_i\rangle\;=&\lim_{M\to\infty}\left(\frac{m}{2\pi\hbar\varepsilon}\right)^{\frac{M}{2}}\int\left(\prod_{k=1}^{M-1}dq_k\right)\\&\times\;\exp\left\{-\frac{\varepsilon}{\hbar}\sum_{k=1}^{M}\left(\frac{m}{2}\left[\frac{q_k-q_{k-1}}{\varepsilon}\right]^2+v\,(q_k)\right)\right\}\\&=\int\limits_{q\,(0)\,=\,x_i}^{q\,(\beta\,\hbar)\,=\,x_i}Dq\,(\tau)\,\exp\left\{-\frac{1}{\hbar}\,S\,[q]\right\},\end{aligned} \tag{3.4}$$

with

$$\int\limits_{q\,(0)\,=\,x_i}^{q\,(\beta\,\hbar)\,=\,x_i}Dq\,(\tau)\;=\;\lim_{M\to\infty}\int\left(\prod_{k\,=\,1}^{M-1}dq_k\right)\,\left(\frac{m}{2\,\pi\,\hbar\,\varepsilon}\right)^{\frac{M}{2}} \tag{3.5}$$

and Euclidean action

$$S\,[q]\;=\;\int\limits_0^{\beta\,\hbar}d\tau\,\left[\frac{m}{2}\,\dot{q}^2\;+\;v\,(q)\right] \tag{3.6}$$

where we have introduced $\dot{q}\;=\;dq/d\tau$ for short. The boundary values are fixed, $q_0\;=\;q_M\;=\;x_i$. The partition function Z as trace in coordinate space can be written as path integral over *all* periodic functions $q\,(\tau)$ of fixed period $\beta\,\hbar$

$$\begin{aligned}Z=\mathrm{Tr}(\mathrm{e}^{-\beta\,H})&=\int dx\,\langle x|\mathrm{e}^{-\beta\,H}|x\rangle\\&=\int dx\int\limits_{q\,(0)\,=\,x}^{q\,(\beta\,\hbar)\,=\,x}Dq\,(\tau)\,\exp\left\{-\frac{1}{\hbar}\,S\,[q]\right\}\\&=\int\limits_{q\,(0)\,=\,q\,(\beta\,\hbar)}Dq\,(\tau)\,\exp\left\{-\frac{1}{\hbar}\,S\,[q]\right\},\end{aligned} \tag{3.7}$$

and the likelihood (2.16) takes the form

$$p(x_T|O_T,\,V)=\prod_i\left\{\frac{\int_{q(0)=x_i}^{q(\beta\hbar)=x_i}Dq(\tau)\exp\left(-\frac{1}{\hbar}S[q]\right)}{\int_{q(0)=q(\beta\hbar)}Dq(\tau)\exp\left(-\frac{1}{\hbar}S[q]\right)}\right\}. \tag{3.8}$$

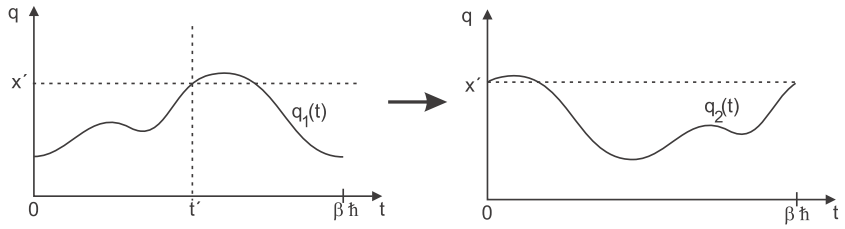

Fig. 1. Equivalent paths $q_1(\tau)$ and $q_2(\tau)$ in the interval $[0,\, \hbar\beta]$, explaining equation (3.12). In the figure τ is denoted t.

In this representation the posterior density reads

$$p(V|D) \sim \int \left(\prod_{i=1}^{N} Dq_i(\tau)\right) \exp\left\{-\frac{1}{\hbar}\sum_{i=1}^{N} F_i[q_i,\, v]\right\} \tag{3.9}$$

with total action

$$F = \sum_i F_i[q_i,\, v] = \sum_i S[q_i,\, v] + N\hbar \ln Z[v] + \frac{\hbar\gamma}{2}\Gamma[v], \tag{3.10}$$

inserting equations (3.4), (3.6), and (3.7) into (2.17) and (2.18). Note that to each data point x_i is assigned its own path integral.

According to (3.7), the functional derivative of Z leads to

$$\begin{aligned}\frac{\delta Z}{\delta v(x')} &= -\frac{1}{\hbar}\int\limits_{q(0)=q(\beta\hbar)} Dq(\tau)\, \exp\left\{-\frac{1}{\hbar}S[q]\right\} \\ &\quad\times \int_0^{\beta\hbar} d\tau'\, \delta(q(\tau') - x') \\ &= -\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau' \int\limits_{q(0)=q(\beta\hbar)} Dq(\tau)\, \exp\left\{-\frac{1}{\hbar}S[q]\right\} \\ &\quad\times \delta(q(\tau') - x'),\end{aligned} \tag{3.11}$$

interchanging the order of integration in the second step. To evaluate the above path integral we observe that action $S[q]$ and measure $Dq(\tau)$ are invariant under cyclic shift of each path $q(\tau)$ around some arbitrary value τ'. This is displayed in Figure 1 where the two paths $q_1(\tau)$, $q_2(\tau)$ cover the same set of values in the interval $[0,\, \beta\hbar]$ and thus generate the same value for the integral $\int d\tau\, v(q(\tau))$. The same reasoning holds for the derivatives $\dot{q}_1$, $\dot{q}_2$, hence $\int d\tau\, (\dot{q}(\tau))^2$ also has the same value for the two paths. Therefore the path integral in (3.11), running over all periodic paths which go through point x' at time τ', can be expressed as the path integral over all paths which start and end at x':

$$\begin{aligned}&\int\limits_{q(0)=q(\beta\hbar)} Dq(\tau)\, \exp\left\{-\frac{1}{\hbar}S[q]\right\} \delta(q(\tau') - x') \\ &= \int\limits_{q(0)=x'}^{q(\beta\hbar)=x'} Dq(\tau)\, \exp\left\{-\frac{1}{\hbar}S[q]\right\} \\ &= \langle x'|\mathrm{e}^{-\beta H}|x'\rangle\ ,\end{aligned} \tag{3.12}$$

using equation (3.1). Note that (3.12) holds independent of the choice of τ'. The remaining integral in (3.11) is then trivial, $\int_0^{\beta\hbar} d\tau' = \beta\hbar$, confirming the expected result

$$\frac{\delta Z}{\delta v(x')} = \frac{\delta}{\delta v(x')}\int dx\, \langle x|\mathrm{e}^{-\beta H}|x\rangle = -\beta\, \langle x'|\mathrm{e}^{-\beta H}|x'\rangle\ . \tag{3.13}$$

In the functional derivative of matrix elements $\langle x_i|\mathrm{e}^{-\beta H}|x_i\rangle$ with respect to v,

$$\begin{aligned}&\frac{\delta}{\delta v(x')}\, \langle x_i|\mathrm{e}^{-\beta H}|x_i\rangle \\ &= -\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau' \int\limits_{q(0)=x_i}^{q(\beta\hbar)=x_i} Dq(\tau)\, \exp\left\{-\frac{1}{\hbar}S[q]\right\} \delta(q(\tau') - x') \\ &= -\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau' \int\limits_{\substack{q(0)=x_i \\ q(\tau')=x'}}^{q(\beta\hbar)=x_i} Dq(\tau)\, \exp\left\{-\frac{1}{\hbar}S[q]\right\},\end{aligned} \tag{3.14}$$

the τ'–integration is nontrivial (see Sect. 6).

With the exact expressions for the basic quantities at hand, we will now study two variants of approximation for solving the inverse problem of quantum statistics. In variant 1 (Sects. 4 and 5) we use the stationary phase approximation for the matrix elements (3.1) of the statistical operator, $\delta S/\delta q_i = 0$, which leads to classical paths of a (fictitious) particle in the (inverted) potential $-v(q)$. We develop an explicit, approximate form of the stationarity equation (2.9) for the posterior (Sect. 4) which is discussed by analogy to the ergodic theorem. Matrix elements of the statistical operator as building blocks for the likelihood are calculated in Section 5, taking into account quadratic fluctuations around the classical paths. For large masses, the classical limit is obtained. Starting point for variant 2 are the exact stationarity equations (2.19) for the posterior in path integral representation, then the following approximations are employed: Statistical operator and partition function are treated in stationary phase approximation, as discussed in Sections 4 and 5. For the respective derivatives with respect to potential V, approximate expressions are developed in Section 6. Variant 2 is more general than variant 1 which turns out to be a special case of variant 2: We will show how to recover the stationarity equation for the posterior of variant 1, and how to improve it.

4 Maximizing the posterior in stationary phase approximation

Following the reasoning in Section 2 for the v-integration we shall treat the integrals (3.4) in stationary phase approximation, looking for paths $q(\tau)$ which minimize the action $S = \sum_i S[q_i, v]$ and account for the main contribution to the integrals. The corresponding stationarity equations,

$$0 = \frac{\delta S}{\delta q_i} = -m\,\ddot{q}_i + \frac{d}{dq_i}\,v(q_i) \quad \text{for} \quad i = 1, \ldots, N \tag{4.1}$$

with boundary conditions

$$q_i(0) = q_i(\beta\hbar) = x_i \tag{4.2}$$

are the classical equations of motion for a fictitious particle of mass m in the inverted potential $-v(q)$ with boundary conditions determined by the data points x_i. Their solutions serve as starting points for a quantum mechanical expansion.

For each path $q_i(\tau)$ the energy

$$E_i = \frac{1}{2}\,m\,\dot{q}_i^2 - v(q_i) \tag{4.3}$$

is conserved. Equations (4.1), (4.2) have to be solved simultaneously with the corresponding approximation of the stationarity equation (2.9), explicitly from (3.10),

$$\begin{aligned} 0 &= \frac{\delta F}{\delta v(x)} \\ &= \sum_{i=1}^{N} \int_0^{\beta\hbar} d\tau\,\delta(q_i(\tau) - x) - \beta\hbar N \langle x|\frac{\mathrm{e}^{-\beta H}}{Z}|x\rangle \\ &\quad + \gamma\hbar \int dx'\,K(x, x')\,(v(x') - v_0(x')) \end{aligned} \tag{4.4}$$

for the choice (2.10) of the prior $p(V)$. This approximation scheme (variant 1) first approximates the path integral in the likelihood and then develops the stationarity equations for the posterior in this approximation ("variation after approximation").

The integral in the first term of (4.4) over δ-distributions can be evaluated, for simple zeroes of the arguments, with the help of equation (4.3),

$$\begin{aligned} \int_0^{\beta\hbar} d\tau\,\delta(q_i(\tau) - x) &= \sum_{j_i=1}^{n_i(x)} \frac{1}{|\dot{q}_i(\tau_{j_i})|} \\ &= \sum_{j_i=1}^{n_i(x)} \frac{1}{\sqrt{\frac{2}{m}\,(E_i + v(q_i(\tau_{j_i})))}} \\ &= \frac{n_i(x)}{\sqrt{\frac{2}{m}\,(E_i + v(x))}}, \end{aligned} \tag{4.5}$$

$n_i(x)$ being the number of times τ_{j_i} with $q_i(\tau_{j_i}) = x$, $0 \le \tau_{j_i} \le \beta\hbar$. The path integrals for the statistical operator and the partition function in the second term of (4.4) will be discussed in detail in the following Section 5.

A compact and instructive form of condition (4.4) is obtained by multiplying with some arbitrary observable $f(x)\,/\,N\,\beta\hbar$ and integrating over x,

$$\begin{aligned} 0 &= \frac{1}{N\,\beta\hbar} \sum_{i=1}^{N} \int_0^{\beta\hbar} d\tau\,f(q_i(\tau)) - \int dx\,f(x)\,\langle x|\frac{\mathrm{e}^{-\beta H}}{Z}|x\rangle \\ &\quad + \frac{\gamma}{N\,\beta} \int dx\,dx'\,f(x)\,K(x, x')\,[v(x') - v_0(x')] \\ &= \frac{1}{N} \sum_{i=1}^{N} \overline{f}_i - \langle f\rangle \\ &\quad + \frac{\gamma}{N\,\beta} \int dx\,dx'\,f(x)\,K(x, x')\,[v(x') - v_0(x')]\,, \end{aligned} \tag{4.6}$$

where $\overline{f}_i$ denotes the mean of f with respect to (imaginary) time τ along path $q_i(\tau)$ and $\langle f\rangle$ the thermal expectation value of observable f. Condition (4.6) reminds of the ergodic theorem of statistical mechanics [9] concerning time and ensemble average, there are, however, differences in three respects:

1. the time average in (4.6) is over a finite interval only,
2. paths $q_i(\tau)$ refer to boundary conditions (4.2) rather than to initial conditions for $q(\tau)$, $\dot{q}(\tau)$, and
3. the prior gives a contribution to (4.6), non-zero in general, in contrast to the ergodic theorem.

In the high temperature limit, $\beta \to 0$, the prior term dominates condition (4.6), as expected, since the first two terms in (4.6) become β-independent. Prior knowledge $p(V)$ completely determines the maximum posterior solution. In contrast, the prior on v becomes negligeable at low temperature, corresponding to large β-values, and the first two terms of (4.6) fulfill the ergodic theorem. In fact, the potential

$$v(x) = -\lim_{a\to\infty} a \sum_{i=1}^{N} \delta(x - x_i) \tag{4.7}$$

is a solution of (4.4), if the prior can be neglected. For the corresponding classical potential $-v(q) = +\lim_{a\to\infty} a \sum_{i=1}^{N} \delta(q - x_i)$ the equations of motion (4.1) with boundary conditions (4.2) have unstable solutions

$$q_i(\tau) = x_i\,, \tag{4.8}$$

and the first term in (4.4) reads

$$\begin{aligned} \sum_{i=1}^{N} \int_0^{\beta\hbar} d\tau\,\delta(q_i(\tau) - x) &= \int_0^{\beta\hbar} d\tau \sum_{i=1}^{N} \delta(x_i - x) \\ &= \beta\hbar \sum_{i=1}^{N} \delta(x_i - x)\,. \end{aligned} \tag{4.9}$$

For large β-values

$$\langle x|\mathrm{e}^{-\beta H}|x\rangle \quad \rightarrow \quad \sum_{i=1}^{N} \langle x|\varphi_{0i}\rangle \langle\varphi_{0i}|x\rangle \mathrm{e}^{-\beta E_0} \qquad (4.10)$$

where the N-fold degenerate quantum ground state $\langle x|\varphi_{0i}\rangle$ is strongly localized by potential $v(x)$, equation (4.7), around the data points x_i such that

$$|\langle x|\varphi_{0i}\rangle|^2 \quad \rightarrow \quad \delta(x - x_i) \qquad (4.11)$$

in proper normalization. Hence, with $Z = \sum_{i=1}^{N} \mathrm{e}^{-\beta E_0} = N\mathrm{e}^{-\beta E_0}$, the second term in (4.4),

$$\frac{1}{Z}\langle x|\mathrm{e}^{-\beta H}|x\rangle \quad \rightarrow \quad \frac{1}{N}\sum_{i=1}^{N} \delta(x - x_i)\,, \qquad (4.12)$$

cancels the first one, equation (4.9).

So far we have restricted ourselves to position measurements. If given data refer to other observables, one can use closure relations to calculate the required matrix elements in those observables while retaining the above path integral formalism. A typical example would be particle momenta rather than positions. In this case, Fourier transformation leads to

$$\begin{aligned}\langle\tilde{p}|\mathrm{e}^{-\beta H}|\tilde{p}\rangle &= \int dx\,dx'\,\langle\tilde{p}|x'\rangle\,\langle x'|\mathrm{e}^{-\beta H}|x\rangle\,\langle x|\tilde{p}\rangle \\ &\sim \int dx\,dx' \int_{q(0)=x}^{q(\beta\hbar)=x'} Dq(\tau)\,\exp\left\{-\frac{1}{\hbar}\Big(S[q] \right. \\ &\quad \left. + i\,\tilde{p}\,(x' - x)\Big)\right\} \\ &= \int Dq(\tau)\,\exp\left\{-\frac{1}{\hbar}\Big(S[q] + i\,\tilde{p}\,\big(q(\beta\hbar)\right. \\ &\quad \left. - q(0)\big)\Big)\right\} \qquad (4.13)\end{aligned}$$

where the integration is over *all* paths $q(\tau)$ of the interval $[0, \beta\hbar]$. Integral (4.13) may then be calculated in saddle point approximation.

5 Quadratic fluctuations around stationary paths and classical limit

To evaluate matrix element

$$\langle x|\mathrm{e}^{-\beta H}|x\rangle = \int_{q(0)=x}^{q(\beta\hbar)=x} Dq(\tau)\,\exp\left\{-\frac{1}{\hbar}S[q]\right\} \qquad (5.1)$$

we start from the stationarity equations (4.1), (4.2). They read, dropping the label i and using $v' = dv/dq_x$ for simplicity of notation,

$$0 = \frac{\delta S}{\delta q} = -m\,\ddot{q} + v'(q) \quad \text{with} \quad q(0) = q(\beta\hbar) = x\,. \qquad (5.2)$$

The stationary solutions $q_x(\tau)$ of (5.2) yield the main contribution to the path integral (5.1); fluctuations around these solutions $q_x(\tau)$ can be taken care of by a variable transformation

$$q(\tau) = q_x(\tau) + r(\tau) \quad \text{with} \quad r(0) = r(\beta\hbar) = 0\,. \qquad (5.3)$$

Assuming that only small deviations of $q(\tau)$ from $q_x(\tau)$ are important for the integral (5.1), we approximate

$$v(q) = v(q_x) + (q - q_x)\,v'(q_x) + \frac{1}{2}(q - q_x)^2\,v''(q_x) \qquad (5.4)$$

and find for the action

$$\begin{aligned}S[q] = &\int_0^{\beta\hbar} d\tau\,\left(\frac{m}{2}\,\dot{q}_x^2 + v(q_x)\right) \\ &+ \int_0^{\beta\hbar} d\tau\,\left(\frac{m}{2}\,\dot{r}^2 + \frac{1}{2}\,v''(q_x)\,r^2\right), \qquad (5.5)\end{aligned}$$

as the term $\int_0^{\beta\hbar} d\tau\left(m\,\dot{q}_x\,\dot{r} + v'(q_x)\,r\right)$ vanishes by virtue of (5.2), (5.3) and partial integration. Fluctuation $r(\tau)$ is thus governed by the curvature of the classical potential, $v''(q_x)$, and the above boundary condition.

For the additive action (5.5) the matrix element (5.1) of the statistical operator factorizes

$$\langle x|\mathrm{e}^{-\beta H}|x\rangle = A_x \exp\left\{-\frac{1}{\hbar}S[q_x]\right\} \qquad (5.6)$$

with

$$\begin{aligned}A_x = &\int_{r(0)=0}^{r(\beta\hbar)=0} Dr(\tau)\exp\left\{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\left(\frac{m}{2}\,\dot{r}^2 + \frac{1}{2}\,v''(q_x)\,r^2\right)\right\} \\ = &\int_{r(0)=0}^{r(\beta\hbar)=0} Dr(\tau)\exp\left\{-\frac{1}{2\hbar}\int_0^{\beta\hbar} d\tau\,d\tau'\,r(\tau')\right. \\ &\left.\times\left(\frac{\delta^2 S[q]}{\delta q(\tau')\,\delta q(\tau)}\bigg|_{q=q_x}\right) r(\tau)\right\} \qquad (5.7)\end{aligned}$$

and Hesse-matrix

$$\begin{aligned}&\frac{\delta^2 S[q]}{\delta q(\tau')\,\delta q(\tau)}\bigg|_{q=q_x} = \\ &\qquad \delta(\tau - \tau')\left(-m\,\frac{\partial^2}{\partial\tau^2} + v''(q_x(\tau))\right)\,, \qquad (5.8)\end{aligned}$$

in approximation (5.4).

The remaining path integral (5.7) can be evaluated by the van Vleck–formula [10]:

$$\langle x|\mathrm{e}^{-\beta H}|x\rangle = A_x \exp\left\{-\frac{1}{\hbar}S[q_x]\right\} = \left(-\frac{1}{2\pi\hbar}\frac{\partial^2 S[q_x]}{\partial x^2}\right)^{\frac{1}{2}} \exp\left\{-\frac{1}{\hbar}S[q_x]\right\}. \tag{5.9}$$

For the partition function Z we use the result (5.9) for the matrix element of the statistical operator

$$Z = \int dx'\, A_{x'} \exp\left\{-\frac{1}{\hbar}S[q_{x'}]\right\}. \tag{5.10}$$

Combining (5.6) and (5.10) results in the normalized matrix element of the statistical operator

$$\langle x|\mathrm{e}^{-\beta H}|x\rangle / Z = \frac{A_x \exp\left\{-\frac{1}{\hbar}S[q_x]\right\}}{\int dx'\, A_{x'} \exp\left\{-\frac{1}{\hbar}S[q_{x'}]\right\}}, \tag{5.11}$$

with the factor A_x comprising quantum fluctuations around the classical path $q_x(\tau)$.

The x'-integral in Z in equations (5.10), (5.11) can either be done numerically or be treated in stationary phase approximation. The action $S[q]$ depends on x through the boundary values of $q(\tau)$, and its derivative with respect to the upper (lower) boundary value of q yields the corresponding momentum ${}^{+}_{(-)}p$. The stationarity condition for S thus poses the additional boundary condition

$$p(\beta\hbar) - p(0) = 0\,. \tag{5.12}$$

Hence one has to find x_0 such that the solutions of the classical equations of motion (4.1) fulfill boundary conditions for both coordinate $q(\tau)$ and velocity $\dot{q}(\tau)$,

$$q(0) = q(\beta\hbar) = x_0 \quad \text{and} \quad \dot{q}(0) = \dot{q}(\beta\hbar)\,. \tag{5.13}$$

Then

$$Z = A_{x_0} \exp\left\{-\frac{1}{\hbar}S[q_{x_0}]\right\} \tag{5.14}$$

in lowest order stationary phase approximation, with A_{x_0} the analogue of A_x.

Two approximations for computing matrix elements (5.6) are of interest. First, for large masses m such that v''/m is small, we may neglect the x–dependence of the fluctuation factor (5.7) which then drops out in the normalized matrix element (5.11),

$$\frac{\langle x|\mathrm{e}^{-\beta H}|x\rangle}{Z} = \frac{\exp\left(-\frac{1}{\hbar}S[q_x]\right)}{\int dx' \exp\left(-\frac{1}{\hbar}S[q_{x'}]\right)} \tag{5.15}$$

in *semiclassical* approximation. Second, in the strict limit $m \to \infty$ the equations of motion (5.2) simplify,

$$\ddot{q}_x = \frac{1}{m}v'(q_x) \to 0 \quad \text{for} \quad m \to \infty\,, \tag{5.16}$$

and are solved by the static paths

$$q_x(\tau) = x, \qquad \dot{q}_x(\tau) = 0 \tag{5.17}$$

for the boundary conditions of (5.2). Then from (5.6)

$$\langle x|\mathrm{e}^{-\beta H}|x\rangle \to A_x \exp(-\beta v(x)) \tag{5.18}$$

where A_x is now strictly x–independent. The well–known result of *classical* statistics,

$$\frac{\langle x|\mathrm{e}^{-\beta H}|x\rangle}{Z} = \frac{\exp(-\beta v(x))}{\int dx' \exp(-\beta v(x'))}, \tag{5.19}$$

is thus reproduced.

6 Approximations for the derivative of matrix elements of the statistical operator with respect to the potential

After the discussion of the statistical operator and of the partition function in Sections 4 and 5, we will now turn to variant 2. While a simple, explicit expression for the derivative of the partition function is already available in (3.13), we still have to discuss the derivative of matrix elements of the statistical operator, equation (3.14).

Three approaches of approximation for the derivative

$$\frac{\delta}{\delta v(x')}\langle x_i|\mathrm{e}^{-\beta H}|x_i\rangle = -\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau' \int_{q(0)=x_i}^{q(\beta\hbar)=x_i} Dq(\tau) \times \exp\left\{-\frac{1}{\hbar}S[q]\right\} \delta(q(\tau') - x') \tag{6.1}$$

are presented. The general strategy is to find approximations such that in the logarithmic derivative of the statistical operator, needed in (2.19), the statistical operator drops out.

In the first approach, we observe that the main contribution to the path integral stems from the stationary path $q_{x_i}(\tau)$, solution of equations (4.1), (4.2). Hence the distribution $\delta(q(\tau') - x')$ *under* the path integral in (6.1) may be replaced by $\delta(q_{x_i}(\tau') - x')$, referring to the stationary path, *in front* of the path integral. In this approximation,

$$\frac{\delta}{\delta v(x')}\langle x_i|\mathrm{e}^{-\beta H}|x_i\rangle = -\frac{1}{\hbar}\left\{\int_0^{\beta\hbar} d\tau' \delta(q_{x_i}(\tau') - x')\right\} \times \int_{q(0)=x_i}^{q(\beta\hbar)=x_i} Dq(\tau) \exp\left\{-\frac{1}{\hbar}S[q]\right\}, \tag{6.2}$$

the first term in the stationarity equation (2.19) takes the form

$$\frac{\frac{\delta}{\delta v(x')}\langle x_i|\mathrm{e}^{-\beta H}|x_i\rangle}{\langle x_i|\mathrm{e}^{-\beta H}|x_i\rangle} = -\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau'\, \delta(q_{x_i}(\tau') - x') \tag{6.3}$$

in agreement with the first term in (4.4). Variant 1 is thus shown to be a special case of variant 2, their difference only affecting the first term of the respective stationarity equations for the maximum posterior.

Our second approach improves (6.3) in a natural way. Introducing the fluctuations around the classical paths according to (5.3) to (5.5), the contribution of the classical action $S[q_{x_i}]$ can be factored out of the path integral before approximation (6.2) is applied. This amounts to modifying the argument of the δ–distribution in (6.3) (see Appendix),

$$\frac{\frac{\delta}{\delta\, v\,(x')}\langle x_i|\mathrm{e}^{-\beta\, H}|x_i\rangle}{\langle x_i|\mathrm{e}^{-\beta\, H}|x_i\rangle} = -\frac{1}{\hbar}\int\limits_0^{\beta\,\hbar} d\tau'\,\delta\left(q_{x_i}\,(\tau') + r_{x_i}\,(\tau') - x'\right) . \quad (6.4)$$

The fluctuations $r_{x_i}(\tau)$ are governed by the curvature of potential $v(q_{x_i}(\tau))$, being solutions of

$$m\,\ddot{r}_{x_i} = v^{''}\,(q_{x_i}\,(\tau))\,r_{x_i} \quad \text{for} \quad r_{x_i}\,(0) = 0 = r_{x_i}\,(\beta\,\hbar)\ . \quad (6.5)$$

In our third approach, the δ–distribution in its spectral representation is kept under the path integral. Following the introduction of the fluctuations of our second approach, one obtains after some lengthy but trivial manipulations (see appendix)

$$\frac{\frac{\delta}{\delta\, v\,(x')}\,\langle x_i|\mathrm{e}^{-\beta\, H}|x_i\rangle}{\langle x_i|\mathrm{e}^{-\beta\, H}|x_i\rangle} = -\frac{1}{\hbar}\int\limits_0^{\beta\,\hbar} d\tau'\,\frac{\exp\left\{-\frac{(q_{x_i}\,(\tau')-x')^2}{2\,\hbar\,R_{x_i}\,(\tau',\,\tau')}\right\}}{\sqrt{2\,\pi\,\hbar\,R_{x_i}\,(\tau',\,\tau')}}. \quad (6.6)$$

Here $R_{x_i}(\tau,\tau')$ is the Green function of the operator $(-m d^2/d\tau^2 + v''(q_{x_i}(\tau))$ with boundary conditions $R_{x_i}(\beta\hbar,\tau') = R_{x_i}(0,\tau') = 0$. The sharp δ–distribution is thus replaced by a smooth Gaussian function, easier to handle in numerical work. Apart from the stationary phase approximation, the only approximation inherent in (6.6) is the assumption (5.4) of small deviations from the classical paths.

To summarize Section 6, the exact variational equations (2.19) can be treated in stationary phase approximation of the relevant quantities ("variation before approximation"), matrix elements of statistical operator and partition function and their derivatives with respect to the potential being available.

7 Numerical case study

In this section we present numerical results for a simple, one-dimensional model, which merely serve to demonstrate that the path integral technique can be used in actual practice within the Bayesian approach to inverse quantum statistics. Restricting ourselves to variant 1 ("variation after approximation"), we will discuss in turn the classical equations of motion (4.1) with boundary conditions (4.2) and the stationarity equations (4.4) of the maximum posterior approximation, which eventually have to be solved simultaneously.

We start with solving the equations of motion for a given potential v. For a numerical implementation we discretize both the time τ, parametrizing some classical path $q\,(\tau)$, and the position coordinate x, upon which the potential $v\,(x)$ depends. The time interval $[0,\,\beta\,\hbar]$ is divided into n_τ equal steps of length

$$\varepsilon = \beta\,/\,n_\tau \quad (7.1)$$

choosing units such that $\hbar = 1$. A path $q\,(\tau)$ is then coded as vector $\vec{q}$ with components $q_k = q\,(\tau_k)$ for $\tau_k = \varepsilon\,k$; $k = 0,\,1,\,\ldots,\,n_\tau$. The potential $v\,(x)$ is studied on an equidistant mesh of size n_x in space, choosing $n_x = n_\tau$. To match the equidistant values of coordinate x to the corresponding values of the classical path $q\,(\tau)$ we may either round up or down the function values q_k or linearly interpolate the potential between equidistant x-values.

In their discretized version, the classical equations of motion of our fictitious particle in potential $-v\,(q)$ read

$$0 = -\frac{m}{\varepsilon^2}\,(q_{k+1} - 2\,q_k + q_{k-1}) + v'\,(q_k)\ ; \quad k = 1,\,2,\,\ldots\,n_{\tau-1}\ , \quad (7.2)$$

and are to be solved with boundary conditions

$$q_0 = x = q_{n_\tau}\ . \quad (7.3)$$

Equations (7.2) and (7.3) amount to solving the matrix equation, for given $v\,(q)$,

$$-\frac{m}{\varepsilon^2}\begin{pmatrix} \frac{\varepsilon^2}{m} & 0 & \cdots & & \cdots & 0 \\ 1 & -2 & 1 & 0\cdots & & 0 \\ 0 & 1 & -2 & 1 & 0 & \cdots \\ \vdots & & & & & \\ 0 & \cdots & & 1 & -2 & 1 \\ 0 & \cdots & & \cdots & 0 & \frac{\varepsilon^2}{m} \end{pmatrix}\begin{pmatrix} q_0 \\ q_1 \\ \vdots \\ q_{n_\tau-1} \\ q_{n_\tau} \end{pmatrix} + \begin{pmatrix} x \\ v'\,(q_1) \\ \vdots \\ v'\,(q_{n_\tau-1}) \\ x \end{pmatrix} \equiv A\,\vec{q} + \vec{t}\,(\vec{q}) = 0 \quad (7.4)$$

which is done by iteration according to

$$\vec{q}^{\,(j+1)} = \vec{q}^{\,(j)} - \eta_q\left(\vec{q}^{\,(j)} + A^{-1}\,\vec{t}\left(\vec{q}^{\,(j)}\right)\right)\ . \quad (7.5)$$

Step length η_q in (7.5) can be adapted during iteration. Having solved (7.4) for various boundary values x_i numerically, we can calculate the likelihood $p\,(x_i|O_i,\,V)$, equation (2.14), in semiclassical approximation (Eq. (5.15)). In order to analyse the quality of the approximation this likelihood can be compared with the classical (Eq. (5.19))

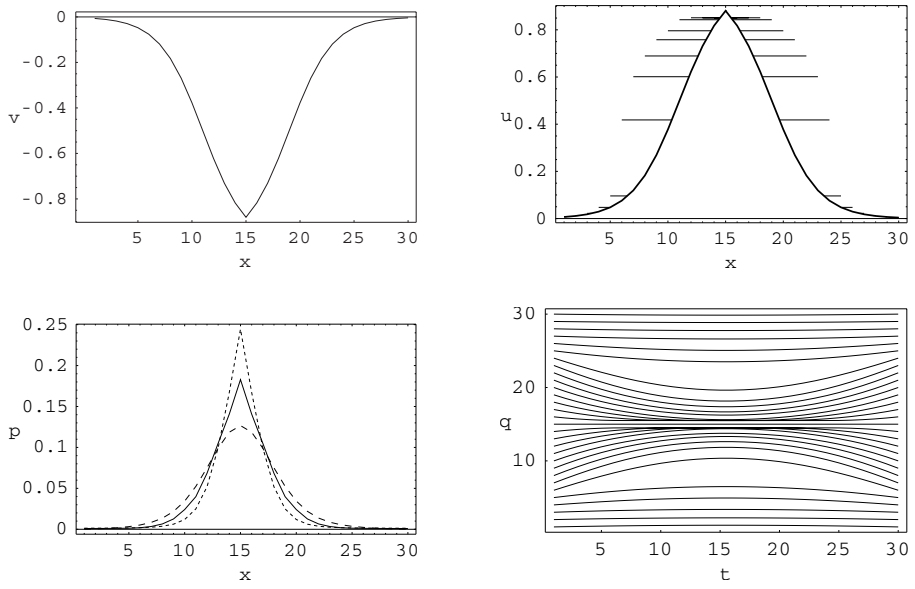

Fig. 2. Comparison of classical, semiclassical and quantum mechanical likelihood for given potential. Upper left part: original potential $v\,(x)$. Upper right part: fictitious potential $u\,(x) = -v\,(x)$, to be used in (7.2); thin horizontal lines indicate range and energy of paths $q_x\,(\tau)$. Lower left part: classical (dotted line), semiclassical (full line) and quantum mechanical (dashed line) likelihoods, see equations (5.19), (5.15) and (7.6), respectively. Lower right part: paths $q_x\,(\tau)$ for various x-values. Parameters used are $m = 0.1$, $\beta = 6$, $n_\tau = 30$, $n_x = 30$. (In the figure τ is denoted t.)

and the exact quantum statistical result [5],

$$p(x_i|O_i, V) = \sum_\alpha \exp\left(-\beta E_\alpha\right)|\phi_\alpha(x_i)|^2/Z,$$
$$Z = \sum_\alpha \exp\left(-\beta E_\alpha\right) \quad (7.6)$$

with ϕ_α the eigenfunctions with energy E_α of the Hamiltonian $H = T + V$.

As example we consider a potential of the form

$$v\,(x) \;=\; -\frac{1}{1 \,+\, \exp\left(\frac{1}{2}\left(|x \,-\, 15| - 4\right)\right)} \qquad (7.7)$$

on an equidistant mesh with $n_x = n_\tau = 30$, shown in Figure 2, upper left part. The right hand side of Figure 2 displays the potential $-v\,(q)$ together with the range and energy of solutions $q_x\,(\tau)$ of (7.4) for various boundary values x (upper part), and the solutions $q_x\,(\tau)$ as functions of τ. Note that solutions $q_x\,(\tau)$ refer to a boundary value problem in the fictitious potential $-v\,(q)$ rather than to the initial value problem of classical mechanics in potential $+v\,(q)$. The probabilities $p\,(x_i|O_i,\, V)$ in the lower left part of Figure 2 exhibit the difference of the classical and semiclassical approximations to the exact quantum statistical result. As expected on account of the uncertainty relation, the variance of the probability distribution increases when going from the classical limit to the exact quantum mechanical calculation. The 3 curves coincide in the classical result, if temperature or mass are increased.

Having finished the preparations of solving the equations of motion we now start searching for numerical solutions of the maximum posterior approximation (4.4). To evaluate the first term of stationarity equation (4.4) for one-dimensional models, one should not use version (4.5): on every one-dimensional, periodic path the velocity takes the value zero for at least one value of τ. A zero of the argument of the δ-distribution at that value of τ will not be a simple one. We have, therefore, for the discretized values τ_k, replaced the value $q\,(\tau_k)$ by the nearest integer of the interval $[0,\, n_x]$, and the δ-distribution in (4.4) by the Kronecker symbol, hence

$$\int d\tau\, \delta\left(q_i\,(\tau) \,-\, x\right) \quad \rightarrow \quad \varepsilon \sum_{j\,=\,1}^{n_\tau} \delta_{q_{ij}\,x}\;. \qquad (7.8)$$

The matrix elements of the second term $\langle x|\exp\left(-\beta\, H\right)|x\rangle/Z$ are calculated semiclassically according to (5.15). Note that this requires to solve the equations of motion (5.2) for every x. In the prior (2.10) we use

$$\Gamma\,[v] \;=\; -\sum_{i,\,j} v_i\, \Delta_{ij}\, v_j \qquad (7.9)$$

with

$$\Delta_{ij} \;=\; \frac{1}{\varepsilon^2} \begin{pmatrix} -2 & 1 & 0 & \cdots & & 0 \\ 1 & -2 & 1 & & & \vdots \\ \vdots & & \cdots & & & \\ & & & \cdots & & \\ & & & & 1 & -2 & 1 \\ 0 & & & \cdots & 0 & 1 & -2 \end{pmatrix}, \qquad (7.10)$$

thus demanding smoothness for the potential $v\,(x)$ to be determined. In our actual calculation we have sampled

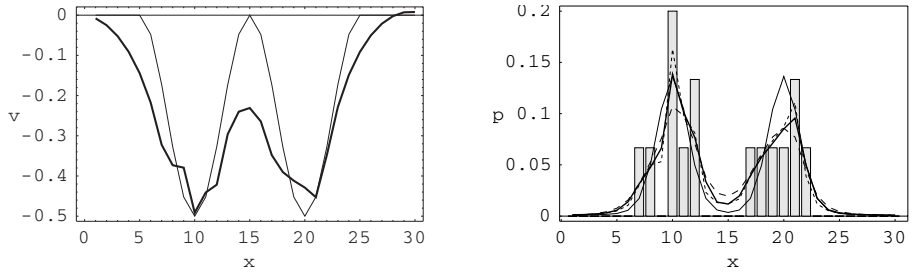

Fig. 3. Bayesian reconstruction of potentials using the path integral method in variant 1 ("variation after approximation"). Left part: original potential (thin line) and reconstructed potential in semiclassical approximation (5.15) (thick line). Right part: relative frequencies of sampled data (bars), likelihood of the true potential (thin line) and of the reconstructed potential (thick line) in semiclassical approximation (5.15). For comparison, classical density (dotted line) and quantum mechanical density (dashed line) according to (5.19) and (7.6) for the reconstructed potential are also shown. Parameters: $\beta = 10$, $m = 1$, $\gamma = 5$, $N = 15$.

$N = 15$ data from the discretized version ($n_x = 30$) of potential

$$v(x) = \begin{cases} \frac{1}{4}\left(\cos\left(\frac{2\pi}{10}(x-15)\right) - 1\right) & \text{for } x \in [5,25] \\ 0 & \text{elsewhere} \end{cases} \tag{7.11}$$

for $\beta = 10$. To this end we first calculated the exact quantum statistical probability distribution (7.6) for the true potential (7.11) and then generated the data by standard sampling techniques. Equation (4.4) is then solved, simultaneously with equations (7.4), (7.5), by iteration, using the gradient descent algorithm according to (2.21). The starting potential for the iteration was the inverted image of the sampled data distribution. Motivation for this choice was the expectation that a high frequency of sampled data implies a deep potential. The hyperparameter γ is chosen such that the depth of the reconstructed potential and of the true potential (7.11) are approximately equal as shown on the left hand side of Figure 3. The right hand side shows the empirical density of data together with the likelihood for the true potential (7.11) and for the reconstructed potential in semiclassical approximation (5.15). In addition the classical and quantum mechanical likelihoods, (5.19) and (7.6), for the above reconstructed potential are presented in this figure. For sufficiently heavy masses the gross shape of the potential is recognized; classical, semiclassical and quantum mechanical likelihoods are approximately the same. With decreasing mass, the differences of classical, semiclassical and quantum mechanical likelihoods become more pronounced, with the double–hump structure of the potential still recognized (Fig. 4). To better reproduce the absolute value of the potential minima one may decrease parameter γ at the expense of distorting the symmetrical shape of the potential, like in Figure 3.

An improvement of the presented results could be achieved, when the x–dependent quadratic correction (5.9) instead of (5.15) is considered. For a numerical implication, the vector $S[q_x]$ has to be calculated for all discretized values x. In a second step the second derivative of $S[q_x]$ with respect to x has to be evaluated by applying the corresponding matrix, as given in (7.10), to the vector $S[q_x]$. As the difference between classical and semiclassical approximations is well pronounced in Figure 2, we have refrained from carrying out the calculation of the quadratic correction (5.9). Furthermore, consistency of the treatment of the quadratic correction and of the choice of the prior would demand to include higher orders of Δ in the inverse covariance K, in order to obtain reliable results for the above second derivative of $S[q_x]$ or the same derivative of $v(q_x(\tau))$ along the classical path.

8 Conclusion

In this paper we have developed the inverse problem of quantum statistics in path integral representation which supplements the energy representation used in a number of recent publications. The advantage of the path integral representation in this context turns out to be twofold: First, one can study the semiclassical and classical limits which are of interest for the analysis of experimental data as obtained from atomic force microscopy. In this rapidly developing field, the unknown force between atoms on the surface of inorganic or organic materials is reconstructed from experimental data on the level of plain classical mechanics [7]. Neither finite temperature nor quantum effects are taken into account although spatial resolution is approaching atomic distances. Second, with the path integral representation for the likelihood and the functional integration over possible potential fields, one obtains a unified description for the basic equations of Bayesian inverse quantum statistics.

Various approximation schemes have been studied for calculating, in this representation, the statistical operator and its derivatives which are the essential quantities in maximum posterior approximation.

Variant 1 applies first the stationary phase approximation to the path integral in the likelihood and then derives, in this approximation, stationarity equations for the posterior. They are to be solved simultaneously with the equations of motion for the classical paths which constitute the stationary phase approximation. Variant 2 starts from the exact stationarity equations for the posterior,

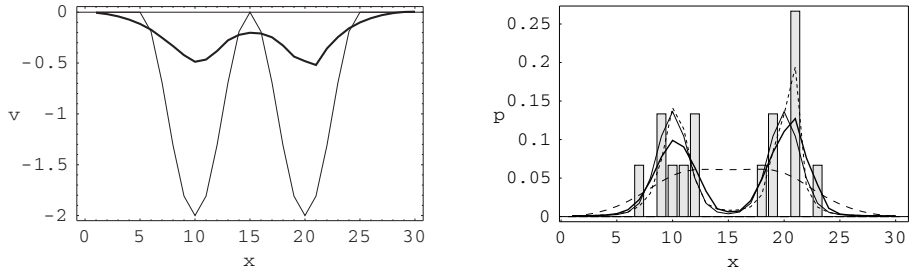

Fig. 4. Bayesian reconstruction of potentials, using the path integral method in variant 1, for small masses: Graphics as in Figure 3, but with parameters: $\beta = 10$, $m = 0.05$, $\gamma = 10$, $N = 15$.

given in terms of matrix elements of the statistical operator and their derivatives with respect to the potential. These quantities are then inserted in stationary phase approximation of the respective integrals. Without going into any detail, it is obvious that variant 2 is superior to variant 1 where the variation of the likelihood is carried out in the restricted variational space spanned by the stationary phase approximation of the path integrals.

Common to both variants are the matrix elements of the statistical operator which, in stationary phase approximation, consist of two factors: one depends exponentially on the action S calculated for the above classical paths; the other takes care of quantum fluctuations around these paths. The latter is given by van Vleck's formula, requiring the second derivative of the action S with respect to the boundary values of the classical paths. In semiclassical and classical approximation, these fluctuation factors may be taken as independent of the boundary values, and then reduce to mere normalization factors which cancel in the likelihood.

The two variants differ in how they treat the derivative of the matrix elements of the statistical oprator with respect to the potential. In variant 1, the derivative of the approximate matrix elements with respect to the potential at position x gives rise to δ–function–type contributions for all times for which the stationary path takes the value x. This result is also obtained in variant 2a when, in the exact derivative, the δ–function under the path integral is approximated by a δ–function referring to the stationary path in front of the path integral. This approximation can be improved by including the fluctuations around the classical paths in the argument of the δ–function (variant 2b). Fluctuations follow from harmonic oscillator equations of motion with time dependent frequency, given by the curvature of the potential along the stationary paths. Finally, keeping the δ–function in its spectral representation under the path integral, an exact, explicit expression is found for the derivative (variant 2c) as long as the fluctuations are treated in harmonic approximation. As a result, the δ–functions of variant 2a, identical with variant 1, are replaced by Gaussians whose widths are given by the Green function of the above oscillator with time dependent frequency.

As to the computational complexities of variant 1 and 2a, respectively, one has to solve N equations of motion for the classical paths in addition to the stationarity equations for the posterior. For the more advanced approaches, variant 2b and 2c, the number of equations of motion to be solved is doubled, adding to the above N equations for the classical paths N more equations for the fluctuations and the Green functions, respectively. While the computational demands for solving these equations are comparable, version 2c is to be preferred being better founded than 2b and easier to handle numerically with its smooth Gaussians versus the sharp δ–functions. A simple numerical example is presented to demonstrate the actual applicability of this approach.

Appendix A

In this appendix details are given to derive formulae (6.4) and (6.6) which improve approximation (6.3) of the logarithmic derivative of the statistical operator. As a first possibility we apply approximation (6.2) to the derivative of the statistical operator after the classical action $S[q_{x_i}]$ has been factored out with the help of the variable transformation (5.3) and the additive form of $S[q]$, equation (5.5). Then,

$$\begin{aligned}
&\frac{\delta}{\delta\, v\,(x')}\,\langle x_i|\mathrm{e}^{-\beta\, H}|x_i\rangle \;=\\
&\qquad -\,\frac{\exp\left\{-\frac{1}{\hbar}\,S\,[q_{x_i}]\right\}}{\hbar}\int\limits_0^{\beta\,\hbar} d\tau' \int\limits_{r\,(0)\,=\,0}^{r\,(\beta\,\hbar)\,=\,0} Dr\,(\tau)\\
&\qquad \times\;\delta\left(q_{x_i}\,(\tau')\,+\,r\,(\tau')\,-\,x'\right)\,\exp\left\{-\frac{1}{\hbar}\,S\,[r]\right\}\\
&= -\frac{\exp\left\{-\frac{1}{\hbar}\,S\,[q_{x_i}]\right\}}{\hbar}\int\limits_0^{\beta\,\hbar} d\tau'\,\delta\left(q_{x_i}\,(\tau')+r_{x_i}\,(\tau')-x'\right)\\
&\qquad\qquad \times \int\limits_{r\,(0)\,=\,0}^{r\,(\beta\,\hbar)\,=\,0} Dr\,(\tau)\,\exp\left\{-\frac{1}{\hbar}S\,[r]\right\} \qquad \text{(A.1)}
\end{aligned}$$

where $r_{x_i}\,(\tau)$ is the solution of

$$m\,\ddot{r}_{x_i} \;=\; v^{''}\left(q_{x_i}\,(\tau)\right)\,r_{x_i} \quad \text{for} \quad r_{x_i}\,(0) \;=\; 0 \;=\; r_{x_i}\,(\beta\,\hbar)\;, \qquad \text{(A.2)}$$

and

$$S\,[r] \;=\; \int\limits_0^{\beta\,\hbar} d\tau\,\left(\frac{1}{2}\,m\,\dot{r}^2\,+\,\frac{1}{2}\,v^{''}\left(q_{x_i}\,(\tau)\right)\,r^2\right)\;. \qquad \text{(A.3)}$$

With (5.6) and (5.7),

$$\langle x_i|\mathrm{e}^{-\beta H}|x_i\rangle = \exp\left\{-\frac{1}{\hbar}S[q_{x_i}]\right\} \times \int_{r(0)=0}^{r(\beta\hbar)=0} Dr(\tau)\exp\left\{-\frac{1}{\hbar}S[r]\right\}, \quad (A.4)$$

one finally has

$$\frac{\frac{\delta}{\delta v(x')}\langle x_i|\mathrm{e}^{-\beta H}|x_i\rangle}{\langle x_i|\mathrm{e}^{-\beta H}|x_i\rangle} = -\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau'\,\delta\left(q_{x_i}(\tau') + r_{x_i}(\tau') - x'\right). \quad (A.5)$$

A second possibility to evaluate the derivative of the statistical operator consists of inserting the spectral representation of the δ-distribution into (6.1). With $q(\tau) = q_{x_i}(\tau) + r(\tau)$ one obtains, in approximation (5.4), for

$$\frac{\delta}{\delta v(x')}\langle x_i|\mathrm{e}^{-\beta H}|x_i\rangle = -\frac{1}{\hbar}\exp\left\{-\frac{1}{\hbar}S[q_{x_i}]\right\}\int_0^{\beta\hbar}d\tau'\int\frac{d\lambda}{2\pi}\exp\{i\lambda(q_{x_i}(\tau')-x')\} \times \int_{r(0)=0}^{r(\beta\hbar)=0} Dr(\tau)\exp\left\{-\frac{1}{\hbar}\int_0^{\beta\hbar}d\tau\Big(\frac{m}{2}\dot{r}^2 + \frac{1}{2}v''(q_{x_i})r^2 - i\lambda\hbar\delta(\tau-\tau')r(\tau)\Big)\right\} \quad (A.6)$$

a path integral where a δ-type potential appears in the action in addition to the harmonic potential with time dependent frequency. Looking for saddle points of the path integral leads to the inhomogeneous equation of motion

$$-m\ddot{r}_{x_i\tau'\lambda}(\tau) + v''(q_{x_i}(\tau))\,r_{x_i\tau'\lambda} = i\lambda\hbar\delta(\tau-\tau') \quad (A.7)$$

with boundary conditions

$$r_{x_i\tau'\lambda}(0) = r_{x_i\tau'\lambda}(\beta\hbar) = 0. \quad (A.8)$$

Note that the solutions of (A.7), (A.8) are both λ- and τ'-dependent. They are intimately related to the Green function $R_{x_i}(\tau,\tau')$ of the operator $-m\frac{d^2}{d\tau^2} + v''(q_{x_i}(\tau))$ with the above boundary conditions,

$$-m\ddot{R}_{x_i}(\tau,\tau') + v''(q_{x_i}(\tau))\,R_{x_i}(\tau,\tau') = \delta(\tau-\tau') \quad (A.9)$$

with

$$R_{x_i}(0,\tau') = R_{x_i}(\beta\hbar,\tau') = 0, \quad (A.10)$$

namely

$$r_{x_i\tau'\lambda}(\tau) = i\hbar\lambda R_{x_i}(\tau,\tau'). \quad (A.11)$$

Furthermore, multiplying (A.7) by $r_{x_i\tau'\lambda}(\tau)$ and integrating over τ, one obtains for the quadratic part of the stationary action of (A.6)

$$-\frac{1}{\hbar}\int_0^{\beta\hbar}d\tau\left(\frac{1}{2}m\dot{r}^2_{x_i\tau'\lambda} + \frac{1}{2}v''(q_{x_i}(\tau))\,r^2_{x_i\tau'\lambda}\right) = -\frac{i\lambda}{2}r_{x_i\tau'\lambda}(\tau') = \frac{\lambda^2\hbar}{2}R_{x_i}(\tau',\tau'). \quad (A.12)$$

Here use has been made of a partial integration, $-\int d\tau\,\dot{r}^2 = \int d\tau\, r\ddot{r}$, and of equations (A.7) and (A.8). After further variable transformation,

$$r(\tau) = r_{x_i\tau'\lambda}(\tau) + l(\tau), \quad (A.13)$$

one finds that in the action of equation (A.6)

$$\int_0^{\beta\hbar}d\tau\Big(m\dot{r}_{x_i\tau'\lambda}(\tau)\dot{l}(\tau) + v''(q_{x_i}(\tau))\,r_{x_i\tau'\lambda}(\tau)\,l(\tau) - i\hbar\lambda\,l(\tau)\,\delta(\tau-\tau')\Big) = \left[m\dot{r}_{x_i\tau'\lambda}(\tau)\,l(\tau)\right]_0^{\beta\hbar} = 0 \quad (A.14)$$

so that (A.6) reads, under approximation (5.4),

$$\frac{\delta\langle x_i|\mathrm{e}^{-\beta H}|x_i\rangle}{\delta v(x')} = -\frac{1}{\hbar}\exp\left\{-\frac{1}{\hbar}S[q_{x_i}]\right\}\int_0^{\beta\hbar}d\tau'\left[\int\frac{d\lambda}{2\pi}\exp\Big\{i\lambda(q_{x_i}(\tau') + r_{x_i\tau'\lambda}(\tau') - x')\Big\}\exp\left\{-\frac{1}{\hbar}S[r_{x_i\tau'\lambda}]\right\}\right] \times \int_{l(0)=0}^{l(\beta\hbar)=0} Dl(\tau)\exp\left\{-\frac{1}{\hbar}S[l]\right\}, \quad (A.15)$$

with abbreviations $S[r_{x_i\tau'\lambda}]$ and $S[l]$ defined according to (A.3). Using (A.12), the integral over λ is of Gaussian type and can be carried out:

$$\int\frac{d\lambda}{2\pi}\exp\left\{i\lambda(q_{x_i}(\tau') + \frac{1}{2}r_{x_i\tau'\lambda}(\tau') - x')\right\} = \int\frac{d\lambda}{2\pi}\exp\left\{i\lambda\,(q_{x_i}(\tau') - x') - \frac{\lambda^2\hbar}{2}R_{x_i}(\tau',\tau')\right\} = \frac{1}{\sqrt{2\pi\hbar R_{x_i}(\tau',\tau')}}\exp\left\{-\frac{(q_{x_i}(\tau')-x')^2}{2\hbar R_{x_i}(\tau',\tau')}\right\}. \quad (A.16)$$

The final result for the logarithmic derivative of $\langle x_i|\mathrm{e}^{-\beta H}|x_i\rangle$ is

$$\frac{\frac{\delta}{\delta v(x')}\langle x_i|\mathrm{e}^{-\beta H}|x_i\rangle}{\langle x_i|\mathrm{e}^{-\beta H}|x_i\rangle} = -\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau' \frac{\exp\left\{-\frac{(q_{x_i}(\tau')-x')^2}{2\hbar R_{x_i}(\tau',\tau')}\right\}}{\sqrt{2\pi\hbar R_{x_i}(\tau',\tau')}}, \tag{A.17}$$

inserting

$$\langle x_i|\mathrm{e}^{-\beta H}|x_i\rangle =$$

$$\exp\left\{-\frac{1}{\hbar}S[q_{x_i}]\right\}\int_{l(0)=0}^{l(\beta\hbar)=0} Dl(\tau)\,\exp\left\{-\frac{1}{\hbar}S[l]\right\} \tag{A.18}$$

according to (5.6) and (5.7). In comparison to the first approach, the δ-distributions in (6.3) and (6.4), equal to (A.5), are replaced in (6.6), or (A.17), by Gaussians which are normalized with respect to x' and whose widths are given by the Green functions $R_{x_i}(\tau,\tau)$. Note that, at least for $v''(q_{x_i}) > 0$,

$$R_{x_i}(\tau',\tau') = \int_0^{\beta\hbar} d\tau \left(\frac{1}{2}m\left(\frac{\partial R_{x_i}(\tau,\tau')}{\partial\tau}\right)^2 + \frac{1}{2}v''(q_{x_i}(\tau))R_{x_i}^2(\tau,\tau')\right) > 0. \tag{A.19}$$

Equation (A.19) follows from (A.9) multiplied by $R_{x_i}(\tau,\tau')$ and integrated over τ. Our result (A.17) does not rest on the assumption about shifting the δ–distribution in front of (6.2) and (A.1), respectively.

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