The Bayesian Inversion Problem for Thermal Average Sampling of Quantum Systems

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Abstract

In this article, we propose a novel method for sampling potential functions based on noisy observation data of a finite number of observables in quantum canonical ensembles, which leads to the accurate sampling of a wide class of test observables. The method is based on the Bayesian inversion framework, which provides a platform for analyzing the posterior distribution and naturally leads to an efficient numerical sampling algorithm. We highlight that, the stability estimate is obtained by treating the potential functions as intermediate variables in the following way: the discrepancy between two sets of observation data of training observables can bound the distance between corresponding posterior distributions of potential functions, while the latter naturally leads to a bound of the discrepancies between corresponding thermal averages of test observables. Besides, the training observables can be more flexible than finite samples of the local density function, which are mostly used in previous researches. The method also applies to the multi-level quantum systems in the non-adiabatic regime. In addition, we provide extensive numerical tests to verify the accuracy and efficiency of the proposed algorithm.

1 Introduction

It has long been a challenging problem to establish inversion theories in quantum canonical ensembles (see Méhats and Pinaud, 2010, Lemm et al., 2000, Lemm, 2000, Lemm et al., 2001, Habeck, 2014, Lemm et al., 2005, Nguyen et al., 2017). One of the difficulties lies in the fact that the quantum canonical ensemble is not directly tractable as the classical case. In this article, the following thermal average of a given observable $\hat{A}$ is of our interest:

$$\langle \hat{A} \rangle = \frac{1}{Z} \text{Tr} \left[ \exp \left( -\beta \hat{H} \right) \hat{A} \right]$$
where $\hat{H} = -\frac{1}{2M} \Delta + V(x)$ is the quantum Hamiltonian, $x \in \mathbb{R}^d$, $M$ is the particle mass, $V(x)$ is the potential function, $\beta$ is referred to as the inverse temperature and $Z \triangleq \text{Tr} \left[ \exp \left( -\beta \hat{H} \right) \right]$ is the partition function. In general, the physical observable $\hat{A}$ corresponds to a self-adjoint operator, whereas for simplicity, we only consider observables as functions of the position variable in this work.

There have been some previous works regarding the existence of such a potential function that yields the local density function $\rho$ exactly as given. In [Méhats and Pinaud, 2010], the authors show that, in a 1-dimensional quantum system with periodic boundary conditions, any positive density function corresponds to a unique density operator minimizing the quantum free energy. Furthermore, the density operator is in the form of $\exp (-(-\Delta + V(x)))$ where $V$ is the chemical potential. The result is extended in [Méhats and Pinaud, 2011] to a multi-dimensional case as well as unbounded domains and non-linear interactions in Hartree or Hartree-Fock systems. On the classical counterpart, [Chayes et al., 1984] addresses the problem whether there exists an external potential corresponding to a given equilibrium single particle density. Results are established for both the canonical and grand canonical distributions. The Hamiltonian concerned is in the form of $H(x_1, x_2, \ldots, x_n) = W(x_1, x_2, \ldots, x_n) + \sum_{i=1}^{n} U(x_i)$ where $W$ is known (not required to be symmetric) and $U$ is unknown. Under a few integrable conditions, $U$ can be uniquely determined by local density function. A following work [Navrotskaya, 2014] extends the conclusion to functions $U$ that may symmetrically contain more than one particle coordinate $x_i$.

Some other works lay emphasis on recovering the potential landscape numerically based on observations to the system. A first work [Lemm et al., 2000] models the likelihood of potential functions based on position observables with finite given eigenvalues and the correspondingly training data $D$, which leads to an expression for the likelihood based on the wave function. Besides, the inversion process is done by maximizing a posteriori which involves taking the variational derivative on the posterior probability and the numerical implementation is based on the gradient descent algorithm. In [Lemm, 2000], the effect of consecutive measurement at non-equilibrium is taken into account. Under the assumption of a time-independent Hamiltonian, the algorithm proposed in the previous work is adapted and amended by considering how the derivative of wave function depends on the time intervals between successive measurements. In [Lemm et al., 2001], the authors discussed how to design priors to recover special properties in potential functions, such as periodicity (as for a distorted crystal surface) or expected discontinuities. A later work [Lemm et al., 2005] rewrites the formula for the thermal average by using the Feynman path integral. To effectively (in numerical sense) evaluate the functional derivative of wave function, the stationary phase approximation is deployed.

The inverse problems in quantum statistics, similarly to those in other fields, can often be ill-posed or highly under-determined. At the same time, there is a wide gap between the works mentioned above: on one side, exact potential functions can be found in certain idealized scenarios, but only on a theoretical level; on the other side, some computational methods have been designed, but there is no clear conclusion on numerical convergence or stability. To merge the gaps, we adopt the Bayesian inversion framework to the quantum thermal average problem. Compared to deterministic approaches for inverse problems, the Bayesian inversion method is more favorable for infinite-dimensional problems (see e.g. [Stuart, 2010], [Dashti and Stuart, 2017]). The advantage of this method is that it does not aim to identify the maximum point of the likelihood, but rather transforms the optimization problem into a sampling problem which naturally provides a statistical result for the inverse problem. There
are a few following works applying this framework, for example, to the determination of the initial condition for Navier–Stokes equation in [Cotter et al., 2010], to a three-dimensional global seismic wave propagation inverse problem with hundreds of thousands of parameters in [Bui-Thanh et al., 2013] and to benchmarks in Higher-Order Ice Sheet Models in [Petra et al., 2014].

The advantages of using this framework are mainly four-fold.

• Firstly, the Bayesian framework views the solution to the inverse problem as a posterior distribution that modifies the a priori knowledge of the unknown by assimilating the noisy observation data. It is impossible to uniquely pinpoint the potential function based on only a finite number of observations, whereas the Bayesian inversion framework admits multiple possible solutions with varying weights described by a posterior distribution. Based on Bayes’s formula, the inversion from the training observations to the posterior distribution has a statistical sense. Furthermore, the stability of the result obtained from the inversion process is also ensured on a theoretical level.

• Secondly, the use of such framework also naturally leads to an efficient numerical algorithm. By building a Markov chain with the posterior distribution as the desired invariant distribution, the potential function can be sampled, providing further predictions on test observations. In the numerical section, we will show that the ground truth of test observations can be recovered if the noise covariance is assumed to be relatively small. This result confirms that not only the posterior distribution is stable with respect to noises, but also the predictions on test observations are practical and meaningful. Besides, the truncation error introduced in the ring polymer representation can be quantitatively estimated, which makes the ring polymer representation a superior asymptotic approximation compared with the static phase approximation adopted in [Lemm et al., 2005].

• Moreover, the restrictions on training observables in this work can be largely relaxed, while in the previous works (see [Lemm et al., 2000] and [Lemm, 2000]) the only viable option is the position observable confined in a small neighborhood of the most likely positions. In the following theorem statement, we will demonstrate that the training and testing observables can be expanded to bounded continuous functions. This greatly helps us to relax the strict requirements applied on practical physical measurements and ensure a wider application in real-life experiments.

• Last but not least, the Bayesian Inversion Framework used in this work also helps build a seamlessly connection between theory and algorithm in the infinite-parameter regime. There are also some other works focusing on problems that share a similar background with this inverse quantum thermal average problem. For example, the inverse Ising problem has been a popular topic. In [Habeck, 2014], the authors adopt the Sequential Monte Carlo algorithm to infer the parameter $\lambda$ in systems with Hamiltonian $E(x) = \sum_{k=1}^{K} \lambda_k f_k(x)$. In [Nguyen et al., 2017], the authors reviewed ways of recovering parameters in the Ising-type Hamiltonian $H(s) = -\sum_i h_i s_i - \sum_{i<j} J_{ij} s_i s_j$. Methods mentioned in these works, however, only apply to a finite-parameter regime. As is emphasized in [Stuart, 2010], avoiding discretization until the last possible moment and valuing the infinite-dimensional nature of the framework enables us to
examine the coherence between theoretical results under the continuum limit and numerical implementation based on the ring polymer representation.

The outline of this paper is listed as follows. In Sec. **2** we review previous works addressing the sampling problem in quantum canonical ensembles. The inversion process theory is established in Sec. **3** the numerical algorithm is proposed in Sec. **4** and a prior analysis is performed in Sec. **5**. After that, we show a few numerical studies in Sec. **6.1**, **6.2** and **6.3** for systems of 1 and 2 levels correspondingly. The numerical tests also help us to verify the theoretical results proposed in Sec. **5** and gain further insights.

2 Review on Quantum Thermal Average

First, we summarize the mathematical model and the numerical approach of the forward problem, i.e. the thermal average of an observable in a quantum system. In the following, we introduce the ring polymer representation of the thermal average, its continuum limit and the path integral molecular dynamics method for numerical simulation.

2.1 Ring polymer representation

The ring polymer representation, first proposed in [Feynman, 1965](Sec. 10) and widely used in chemical physics (e.g. see Sec. 2.9 in [Kleinert, 2009]), approximates the thermal average of observable $\hat{A}$ with respect to the classical Gibbs distribution in the $dN$-dimensional space for ring polymer $q = (q_1, \ldots, q_N) \in \mathbb{R}^{dN}, q_i \in \mathbb{R}^d$ as

$$
\langle \hat{A} \rangle = \frac{1}{Z_N} \int_{\mathbb{R}^{dN}} \left[ \frac{1}{N} \sum_{i=1}^{N} A(q_i) \right] e^{-S_N(q)} dq + O(N^{-2}),
$$

where the action is given by

$$
S_N(q) \triangleq \beta_N \sum_{i=1}^{N} \left[ \frac{M |q_i - q_{i+1}|^2}{2\beta_N^2} + V(q_i) \right]
$$

and $Z_N \triangleq \int_{\mathbb{R}^N} e^{-S_N(q)} dq$ is the normalization constant and $\beta_N \triangleq \beta/N$.

Define the shorthand notation $\overline{A}(q) \triangleq \frac{1}{N} \sum_{i=1}^{N} A(q_i)$. Eqn. 1 indicates that the thermal average $\langle \hat{A} \rangle$ can be approximated by the expectation of $\overline{A}(q)$ with respect to the following Gibbs distribution

$$
\pi^V_N(dq) \triangleq \frac{1}{Z^V_N} e^{-S_N(q)} dq.
$$

However, since the dimension of the configuration space is $dN$, a direct numerical integration based on $\pi^V_N$ is too expensive due to large $N$ required by reducing the approximation error. To avoid the curse of dimensionality, a few numerical sampling methods are designed to approximate the integration by averaging a time series based on Eqn. 3 we will further discuss this topic in Sec. 2.3.
2.2 Continuum limit

As the division number $N$ approaches infinity, there is a formal limit for the ring polymer configuration $q$ as well for the action $S_N$. For given bead number $N$, a piece-wise linear path $q_N$ can be constructed by setting $q_N(j\beta_N) = q_j$ and periodic on $[0, \beta]$, so the formal limit of $q_N$ as $N \to \infty$ is also in the space $L^d = \{q : [0, \beta] \to \mathbb{R}^d, q(0) = q(\beta)\}$. The corresponding limit for the action is given by

$$S(q) \triangleq \int_0^\beta \left[ \frac{M}{2} |\dot{q}|^2 + V(q(\tau)) \right] d\tau,$$

so the thermal average, taking the limit $N \to \infty$, can be formally written as

$$\langle \hat{A} \rangle = \frac{1}{Z} \int_{L^d} \left[ \frac{1}{\beta} \int_0^\beta A(q(\tau)) d\tau \right] \exp(-S(q)) D[q]$$

(4)

where $D[q]$ denotes integration over all paths $q$ with $q(0) = q(\beta)$ and $Z \triangleq \int_{L^d} e^{-S(q)} D[q]$ is the normalization constant.

Eqn. (4) allows us to define the following formal Gibbs distribution (also see [Feynman, 1965] Sec.10 and [Lu and Zhou, 2018b]) on the configuration space

$$\pi^V(dq) \triangleq \frac{1}{Z} \exp(-S(q)) D[q]$$

(5)

so that the thermal average in Eq. (4) can be rewritten as

$$\langle \hat{A} \rangle = \mathbb{E}_{\pi^V(dq)} \left[ \frac{1}{\beta} \int_0^\beta A(q(\tau)) d\tau \right] = \mathbb{E}_{\pi^V(dq)} \overline{A}[q]$$

(6)

where the shorthand notation is defined as

$$\overline{A}[q] \triangleq \frac{1}{\beta} \int_0^\beta A(q(\tau)) d\tau.$$

(7)

Note. To emphasize the dependency of $\langle \hat{A} \rangle$ on the potential $V$, we use the notation $G^A(V)$ referring to the mapping from $V$ to the thermal average $\langle \hat{A} \rangle$ where needed.

2.3 Under-damped Langevin sampling

To enhance the efficiency of the sampling process, an auxiliary momentum variable $p \in \mathbb{R}^{dN}$ with artificial mass $M$ can be introduced. In the augmented state space of position and momentum of ring polymer beads, the thermal average is given by

$$\langle \hat{A} \rangle = \frac{1}{Z_N} \int_{\mathbb{R}^N} \int_{\mathbb{R}^{dN}} \left[ \frac{1}{N} \sum_{i=1}^N A(q_i) \right] e^{-\beta_N H_N(q,p)} dq dp + \mathcal{O}(N^{-2})$$
where the Hamiltonian is given by

$$H_N(q,p) = \frac{1}{2M} |p|^2 + \sum_{i=1}^{N} \left[ \frac{M |q_i - q_{i+1}|^2}{2\beta_N} + V(q_i) \right].$$

(8)

Therefore the classical Gibbs distribution in the extended phase space can be sampled by evolving the following dynamic system:

$$\begin{cases}
\frac{dq}{dt} = \nabla_p H_N dt \\
\frac{dp}{dt} = -\nabla_q H_N dt - \gamma p dt + \sqrt{2\gamma M / \beta_N} dB.
\end{cases}$$

(9)

To numerically integrate the SODE in Eqn. 9, we use the BAOAB method which is proposed in [Leimkuhler and Matthews, 2013a], further tested and compared against other variants (ABOBA and OBABO) in [Leimkuhler and Matthews, 2013b] and [Liu et al., 2016], and investigated elaborately and shown useful for other types of thermostats in [Zhang et al., 2017].

2.4 Multi-level system

The thermal average of a given observable in a multi-level system has been explored in the previous works. In [Menzeleev et al., 2014], kinetically-constrained RPMD is proposed to directly simulate electronically non-adiabatic chemical processes. In [Ananth, 2013], the authors proposed mapping-variable RPMD which constructs continuous Cartesian variables for both electronic states and nuclear degrees of freedom; see also the review paper [Stock and Thoss, 2005].

Recently, a few works focus on the exact computation of multi-level systems. In [Liu and Liu, 2018], three splitting schemes for the Boltzmann operator in the non-adiabatic representation are discussed in detail and multi-electronic-state PIMD is derived afterwards. In [Tao et al., 2018], a corresponding isomorphic Hamiltonian is introduced to fully recover the exact quantum Boltzmann distribution under the Boltzmann sampling with classical nuclear degrees of freedom. In this paper, we implement the method proposed by [Lu and Zhou, 2017] where the non-adiabatic effect is added into consideration by modeling the surface hopping procedure as a Q-process. A following work [Lu and Zhou, 2018a] improves this method by introducing a multiscale integrator for the infinite swapping limit. We will supply the essential formula in Sec. B in the Appendix.

3 Inversion Process Based on Thermal Averages

Sec. 2 has established the forward problem, i.e. given observable $\hat{A}$ and potential $V$, the thermal average can be formulated as

$$y_{\text{truth}} = G^A(V).$$

However, an observation $y$ from the real world or experiment may deviate from the ground truth $G^A(V)$ because of noise, possibly due to instrumental bias, measurement error, and thermal fluctua-
A simplest model for the noise $\eta$ is the additive assumption, i.e.

$$y = G^A(V) + \eta,$$  \hspace{1cm} (10)

and the noise $\eta$ is assumed independent of the potential function $V$. Since $\eta$ is a random variable, a determinate result for the “best” $V$ barely makes sense. Nevertheless, it is sensible to presume a posterior distribution $\mu^y(dV)$ of $V$ based on the noisy observation $y$, given a known prior distribution on the space of all admissible potential functions. As the observable $\hat{A}$ is used to recover the posterior distribution, we will name it as the “training observable”. On the other hand, we in practice are interested in the inference of other thermal averages within the same ensemble, which can be viewed as a weak version of the inverse problem in quantum statistics. Such concern can be generalized to the thermal average of another observable $\hat{O}$, named as the “testing observable”.

Although the prediction from $y$ to $\langle \hat{O} \rangle$ may look like a classical statistics learning problem, the difficulty lies in the nonlinear nature of density operators with respect to the potential function and the observation data in quantum canonical ensembles. To address this both theoretically and numerically, we replace the inverse mapping with the posterior distribution $\pi^y(dy)$, where the weights are obtained by sampling the posterior distribution $\mu^y(dV)$ induced by the noisy training observation. In fact, the weighted-average $\mathbb{E}_{\mu^y(dV)} G^O(V)$ sampled by the algorithm can be written into $\mathbb{E}_{\pi^y(dy)} \hat{O}[q]$, thus it suffices to study the property of the posterior distribution $\pi^y(dy)$ of the conditional variable $q|y$.

In the following sections, we discuss the following properties of the posterior distribution:

**Existence** We formulate the inverse problem in this section. The posterior distribution $\mu^y(dV)$ can be obtained from the prior distribution $\mu_0(dV)$ by evaluating the negative log potential $\Phi(V;y)$ with the training observation $y$. To further describe the conditional variable $q|y$, we can view $V$ as an intermediate variable to obtain the posterior distribution $\pi^y(dy)$ based on the two conditional variables $V|y$ and $q|V$. By the end $\mathbb{E}_{\mu^y(dV)} G^O(V) = \mathbb{E}_{\pi^y(dy)} \hat{O}[q]$, thus it is proved to confirm the consistency between our model and algorithm.

**Solvability** We demonstrate how to numerically sample the posterior distribution $\mu^y(dV)$ and discuss some details in implementation in Sec. 4. The algorithm is an iterative procedure in a proposal-decision approach: in each iteration, a new potential proposal $\hat{V}^{(k+1)}$ is drawn based on the previous sample $V^{(k)}$ and the acceptance probability is based on the comparison between current and previous observation errors. To be more specific, the algorithm can be abstracted as:

**Initialization** Obtain the ground truth observation $y^*$. Draw $\hat{V}^{(0)} = V^{(0)} \sim \mu_0(dV)$.

**Proposal** Draw $\hat{V}^{(k+1)}$ based on $V^{(k)}$. Compute training observation $\hat{y}^{(k+1)} = G^A(\hat{V}^{(k+1)})$.

**Decision** With probability $a\left(\hat{y}^{(k+1)}, y^{(k)}; y^*\right)$ which is consistent with the proposal scheme, accept, otherwise reject the proposal.

Accept $V^{(k+1)} = \hat{V}^{(k+1)}$ and $y^{(k+1)} = \hat{y}^{(k+1)}$.

Reject $V^{(k+1)} = V^{(k)}$ and $y^{(k+1)} = y^{(k)}$. 

8
Stability We give some stability analysis in Sec. 5. We construct a series of proofs to show that the posterior distributions are stable under the disturbance of the noisy observation data.

The formulation of the inverse problem and the stability result will be discussed under the continuum limit, while the numerical scheme are based on the ring polymer representation in finite dimensions. Also, we assume the technical condition that the posterior distribution mentioned in the paper is absolutely continuous to the corresponding prior distribution (e.g. $q|V$ to $q$, $V|y$ to $V$).

3.1 Notations
Without loss of generality, we assume that the physical space of the quantum particle is one-dimensional, i.e. $d = 1$.

The space of $\beta$-periodic loops $q$ (in the continuum limit sense) is defined as

$$X \triangleq \mathcal{L}\mathbb{R} \triangleq \{q : [0, \beta] \to \mathbb{R}, q(0) = q(\beta)\}.$$  

The training observations $y$ based on $N_T$ observables are in the space

$$Y \triangleq \mathbb{R}^{N_T}.$$  

The admissible potential functions $V$ are in the space

$$W^1 \triangleq \left\{V : \left(V - \frac{1}{2}x^2\right) \in L^\infty(\mathbb{R}) \cap L^2(\mathbb{R})\right\}.$$  

To simplify the notation, we refer to $\frac{1}{2}x^2$ as $V_0$.

Since the Hermite basis function (see Section A in Appendix for definition) is a complete orthogonal basis for $L^2(\mathbb{R})$, any given element $V \in W^1$ can be written as the linear combination of the basis as

$$V = V_0 + \sum_{i=0}^{\infty} v_i \phi_i,$$  

where $v_i = \langle V - V_0, \phi_i \rangle$ is the coefficient of the $i$-th basis. By Eqn. 11 we have a mapping from the space of weight sequences $\{v_i\}$ to $W^1$.

To make $W^1$ a Banach space, we endow it with norm

$$||V||_{W^1} \triangleq ||V - V_0||_{L^2} + ||V - V_0||_{L^\infty}.$$  

Then $W^1$ is complete (see Lem. 8 for proof).

In the numerical implementation, we use the truncated version of $W^1$, defined as

$$W^1_L \triangleq \{V : (V - V_0) \in \text{span} (\phi_0, \ldots \phi_L)\}.$$
Therefore, there exists a projection $\Pi^1_L$ of truncation from $W^1$ to $W^1_L$, namely

$$\Pi^1_L(V) = V_o + \sum_{i=0}^L (V - V_o, \phi_i) \phi_i.$$ 

Now $X, Y, W^1$ are Banach spaces endowed with proper norms. To further discuss the relation between variables on these spaces, we need to define a few measures as the prior and posterior distributions.

By Eqn. 5, a given potential function $V$ can induce a formal Gibbs distribution $\pi^V(dq)$ on the position configuration space $X = \mathbb{R}^L$. Especially, we denote $\pi^V_0$ as $\pi_0$. The connection between $\pi_0$ and $\pi^V$ is can be derived from the action $S(q) = \int_0^\beta \left( \frac{M}{2} |\dot{q}|^2 + V(q(\tau)) \right) d\tau$, i.e.

$$\pi^V(dq) \propto \pi_0(dq) \exp \left( -\int_0^\beta \dot{V} \circ \dot{q} d\tau \right)$$

where $\dot{V} \triangleq V - V_o = V - \frac{1}{2}x^2$.

We regard the measure $\pi_0$ induced by the harmonic oscillation potential $V_o$ as the prior on $X$, while $\pi^V$ is the posterior distribution which is absolutely continuous to $\pi_0$. The Radon-Nikodym (R-N for short) derivative $\exp \left( -\int_0^\beta \dot{V} \circ \dot{q} d\tau \right)$ can be viewed as a ‘correction’ to the prior, adding more weight where the correction potential $\dot{V}$ is low.

To give a prior distribution on the potential function space $W^1$, we construct each potential function $V$ from its component $v_i$ in the way that

$$v_i = \gamma_i \xi_i, \quad \xi_i \overset{i.i.d.}{\sim} \mathcal{N}(0, 1)$$

where $\{\gamma_i\}$ is a fixed decaying sequence. This form naturally leads to a Gaussian measure $\mu_0(dV)$ on $W^1$, which is defined by the mean value $V_o$ and the covariance operator

$$\Gamma_V(V, V') \triangleq \sum_{n=0}^\infty \langle V - V_o, \phi_n \rangle \langle V' - V_o, \phi_n \rangle.$$ 

Now we turn to the space of training observations $Y$. Assuming that the noise $\eta$ is a Gaussian noise with mean 0 and positive-definite covariance matrix $\Gamma_\eta \in \mathbb{R}^{NT \times NT}$, the distribution of $\eta$ is clearly $\mathcal{N}(0, \Gamma_\eta)$. By the additive noise assumption, the training observation $y$ is a translation of the ground truth $G^A(V)$, so the distribution of $y$ is $\mathcal{N}\left(G^A(V), \Gamma_\eta\right)$ if the potential function $V$ is fixed.

To sum up, we denote $\tau_0 \triangleq \mathcal{N}(0, \Gamma_\eta)$ as the prior distribution and $\tau^V \triangleq \mathcal{N}\left(G^A(V), \Gamma_\eta\right)$ as the posterior distribution dependent on $Y$.

### 3.2 Formulation: the inversion process

Recall that the goal is to sample the potential function $V$ as well as the testing observable. As we have stated in the beginning of this section, it is equivalent to obtain the weighted average either by sampling $G^O(V)$ from $\mu^y(dV)$ (i.e. the algorithm’s perspective) or by sampling $\mathcal{O}[q]$ from $\pi^y(dq)$ (i.e.
viewing $V$ as an intermediate variable). To describe the posterior distribution $\pi_y (dq)$, it is essential to start from the two conditional variables $V|y$ and $q|y$. In the following reasoning, we establish the posterior distribution $\mu_y (dV)$ of $V|y$ in Eqn. 17 and show that the posterior distribution of $q|y$ is

$$p(q|y) dq = \int_{W^1} \left[ \mu_y (dV) \pi_V (dq) \right].$$

As we have assumed, the training observation $y$ is a noisy version of the exact value $G^A (V)$. Recall that, the noise $\eta$ is independent of $V$ and the distribution of $\eta$ is $\tau_0 = \mathcal{N} (0, \Gamma_\eta)$, so according to Eqn. 10, the conditional distribution of $y|V$ is

$$\tau^V = \mathcal{N} (G^A (V), \Gamma_\eta), \quad (13)$$

merely a translation of $\tau_0$. Consider the joint probability density for $(q, y, V)$:

$$p(q, y, V) = p(q, y|V) p(V) = p(q|V) p(y|V) p(V)$$

the second equation holds since the two conditional variable $q|V$ and $y|V$ are clearly independent. So by using the Bayes’s formula at the starred equation, we have

$$p(q, V|y) = \frac{p(q, y, V)}{p(y)} = \frac{p(q|V) p(y|V) p(V)}{p(y)} = p(q|V) p(V|y). \quad (14)$$

By taking integrals on both sides of Eqn. 14 on $W^1$, we have

$$p(q|y) = \int_{W^1} p(q, V|y) dV = \int_{W^1} p(q|V) p(V|y) dV. \quad (15)$$

We have known that the distribution of $q|V$ is $\pi_V$ as in Eqn. 12. For $V|y$, since the R-N derivative for $\tau^V$ with respect to $\tau_0$ is

$$\frac{d\tau^V}{d\tau_0} (y) = \exp \left( -\frac{1}{2} \left| \Gamma^{-\frac{1}{2}}_\eta \left( y - G^A (V) \right) \right|^2 \right) \exp \left( -\frac{1}{2} \left| \Gamma^{-\frac{1}{2}}_\eta y \right|^2 \right),$$

thus the negative log likelihood can be defined as

$$\Phi (V; y) \triangleq \frac{1}{2} \left| \Gamma^{-\frac{1}{2}}_\eta \left( y - G^A (V) \right) \right|^2 - \frac{1}{2} \left| \Gamma^{-\frac{1}{2}}_\eta y \right|^2 = -\log \left( \frac{d\tau^V}{d\tau_0} (y) \right).$$
By Thm. 16 the conditional distribution of $V | y$ is

$$
\mu^y (dV) \triangleq \mu_0 (dV) \frac{1}{Z (y)} \exp (-\Phi (V; y)) \tag{17}
$$

where $Z (y) \triangleq \int_{W^1} \exp (-\Phi (V; y)) \mu_0 (dV)$ is the partition function.

To sum up, we denote $\pi^y$ as the posterior distribution of $q | y$ obtained from 16 and 17, i.e.

$$
\pi^y (dq) = \int_{W^1} \left[ \mu^y (dV) \pi^V (dq) \right]. \tag{18}
$$

As we have assumed, the posterior distributions $\mu^y$ and $\pi^V$ are absolutely continuous with respect to the prior distributions $\mu_0$ and $\pi_0$ correspondingly, so the absolute continuity of $\pi^y$ with respect to $\pi_0$ holds from Eqn. 18. Moreover, we will give the R-N derivative as follows without proof.

**Lemma 1.** The R-N derivative of the posterior distribution $\pi^y$ w.r.t. the prior distribution $\pi_0$ is

$$
\frac{d \pi^y}{d \pi_0} (q) = \int_{W^1} \left[ \frac{d \mu^y}{d \mu_0} (V) \frac{d \pi^V}{d \pi_0} (q) \mu_0 (dV) \right]. \tag{19}
$$

With these posterior distribution established, now we can examine the coherence between our model (sampling $\mathcal{O} [q]$ from $\pi^y (dq)$) and algorithm (sampling $G^O (V)$ from $\mu^y (dV)$) by the following proposition.

**Proposition 2.** The following two weighted averages are the same:

$$
\mathbb{E}_{\mu^y (dV)} G^O (V) = \mathbb{E}_{\pi^y (dq)} \mathcal{O} [q].
$$

**Proof.** The proof requires no more than a direct calculation: by definition of $\mu^y (dV)$ and $G^O (V)$ we have

$$
\mathbb{E}_{\mu^y (dV)} G^O (V) = \int_{W^1} \mu^y (dV) \left[ \int_{X} \pi^V (dq) \mathcal{O} [q] \right].
$$

On the other hand, by interchanging the order of integrals and definition of $\pi^y (dq)$, we have

$$
\int_{W^1} \mu^y (dV) \left[ \int_{X} \pi^V (dq) \mathcal{O} [q] \right] = \int_{X} \mathcal{O} [q] \left[ \int_{W^1} \mu^y (dV) \pi^V (dq) \right]
$$

$$
= \int_{X} \mathcal{O} [q] \pi^y (dq)
$$

$$
= \mathbb{E}_{\pi^y (dq)} \mathcal{O} [q].
$$

So we arrive at $\mathbb{E}_{\mu^y (dV)} G^O (V) = \mathbb{E}_{\pi^y (dq)} \mathcal{O} [q]$. \qed
4 The Inversion Algorithm

In this section, we will introduce an inversion algorithm for the thermal average sampling in the single level quantum system. Recall that our interest lies in the conditional variable \( q|y \), described by

\[
p(q|y) = \int_{W^1} p(q|V) p(V|y) \, dV
\]

in which the potential \( V \) is viewed as an intermediate variable. Therefore, by making use of the PIMD method (Sec. 2) to sample \( q|V \) and the posterior distribution sampler (Sec. C.4 in Appendix) to sample \( V|y \), the inversion algorithm can sample the conditional variable \( q|y \) as well as the testing observation \( G^O(V)|y \).

4.1 Algorithm overview

The algorithm is mainly two-staged: the first stage is to sample a fixed potential function \( \hat{V}(k) \) proposed by the prior distribution and obtain the \( k \)-th training thermal average \( y(k) = GA(\hat{V}(k)) \) based on path integral molecular dynamics; at the second stage, the average \( y(k) \) is compared against the ground truth \( y^* \) and previous sample \( y(k-1) \), where Metropolis-Hasting method is used to decide whether to keep the proposed \( \hat{V}(k) \) or not. By this way, the conditional variable \( V|y^* \) can be sampled accurately up to the error in PIMD simulations.

4.2 Algorithm implementation

4.2.1 PIMD solver (Line 5 in Alg. 1)

To efficiently solve the forward problem, we implement a PIMD solver in C++ and perform tests on a machine equipped with a Intel Core i5-7300HQ (single-threaded at 3.5GHz).

4.2.2 Metropolis Hasting method (Line 10 in Alg. 1)

The measure of interest \( \mu^y \) is absolutely continuous with respect to \( \mu_0 \) and its R-N derivative is in proportion to \( \exp(-\Phi(V;y)) \). So in order to sample \( \mu^y \) based on proposals from \( \mu_0 \), according to Assu. 20, the decision function can be chosen as

\[
a(V_{old} \rightarrow V_{new}) = \exp(\min\{0, \Phi(V_{old}) - \Phi(V_{new})\})
\]

so that the detailed balance condition will be satisfied as long as the proposal kernel is reversible with respect to the prior distribution.
Algorithm 1 Inversion Sampler For 1-Level Quantum Thermal Average Problem

1: Initialize the potential function $V^{(0)} = \hat{V}^{(0)}$ (one choice is the harmonic potential $V_o$) and the noise covariance matrix $\Gamma_\eta$.
2: Obtain the ground truth of training observation $y^*$ (with or without noise).
3: Set $k = 0$.
4: while stopping condition is not satisfied (e.g. $k < K_{total}$) do
5: Sample a sequence of bead configurations $q_1, \ldots, q_{N_1}$ distributed according to the measure $\pi \hat{V}^{(k)}$ induced by the proposed potential function $\hat{V}^{(k)}$.
6: Average the observations $A(q_i)$ to obtain the $k$-th training observation $\hat{y}^{(k)} = \frac{1}{N_1} \sum_{i=1}^{N_1} A(q_i)$. (Note: $y^{(0)} = \hat{y}^{(0)}$)
7: Compute the negative log likelihood \[
\hat{\Phi}^{(k)} \triangleq \Phi \left( \hat{V}^{(k)}; y^* \right) = \left\langle \hat{y}^{(k)}; \Gamma_\eta^{-1} \left( \frac{1}{2} \hat{y}^{(k)} - y^* \right) \right\rangle.
\]
8: if $k > 0$ then
9: Pick a random number $r^{(k)} \sim \mathcal{U}[0, 1]$.
10: if $r^{(k)} < \exp \left( \min \left[ 0, \Phi^{(k-1)} - \hat{\Phi}^{(k)} \right] \right)$ then
11: Accept the proposal: $V^{(k)} = \hat{V}^{(k)}$, $y^{(k)} = \hat{y}^{(k)}$ and $\Phi^{(k)} = \hat{\Phi}^{(k)}$.
12: else
13: Reject the proposal: $V^{(k)} = V^{(k-1)}$, $y^{(k)} = y^{(k-1)}$ and $\Phi^{(k)} = \Phi^{(k-1)}$.
14: end if
15: end if
16: Store the decided potential function $V^{(k)}$.
17: Obtain thermal average $G^O \left( V^{(k)} \right)$ of test observables if needed.
18: Propose $\hat{V}^{(k+1)}$ based on $V^{(k)}$.
19: end while
4.2.3 Proposal kernel of potential function (Line 18 in Alg. 1)

The next step is to choose a proposal kernel which is reversible with respect to the prior distribution. Recall that each potential function \( V \) in the truncated space \( W_L^1 \) can be expressed as

\[
V = V_o + \sum_{i=0}^{L} \xi_i \gamma_i \phi_i
\]

while the covariance operator \( \Gamma_V (\Pi_L^1, \Pi_L^1) \) has the corresponding truncated form \( \text{diag} (\gamma_0^2, \ldots, \gamma_L^2) \), so to propose \( V \) is essentially to propose \( \{\xi_i\}_{i=0}^L \).

However, a direct random uniform proposal regardless of previous samples will lead to unaffordable rejections rates, which is often caused by the small scale of the noise covariance operator \( \Gamma_\eta \). To lower the rejection rate, we can take the advantage of the fact that the prior distribution of interest is Gaussian and implement a simple but efficient proposal generator, which ensures that two successive proposals are close to keep the negative log potential \( \Phi \) flowing in a smoother way and also keeps the invariant distribution unchanged. For the algorithms in detail, we refer Section D in Appendix and [Cotter et al., 2012] for the readers.

4.2.4 Regularity of \( V \in W^1 \)

Recall that elements in \( W^1 \) can be expressed in the form of

\[
V = V_o + \sum_{i=0}^{\infty} \xi_i \gamma_i \phi_i
\]

where \( \{\xi_i\} \) are the random variables and \( \{\phi_i\} \) is the basis. In particular, the decaying sequence \( \{\gamma_i\} \) serves as a parameter controlling the regularity of \( V \). We assume that, given a constant parameter \( \beta \in (0, 1) \), the asymptotic behavior of \( \{\gamma_i\} \) is given by

\[
\gamma_i = O(i^{-s}), \quad s > \max \left\{1, \frac{\beta + 2}{4(1 - \beta)} \right\}.
\]

Under such assumption, we have the following properties:

1. The exponent \( s \) is larger than 1, so by Prop. [11] \( V - V_o \) is in \( L^\infty \cap L^2 \) and \( V \) is in \( W^1 \).
2. The exponent \( s \) is larger than \( \frac{\beta + 2}{4(1 - \beta)} \), so by Prop. [12] \( V \) has \( \beta \)-order Hölder continuity.

5 Stability Analysis

In terms of stability, recall that the variable of interest is \( q|y \) in distribution of \( \pi^y \), so we want to establish a continuous dependency of \( \pi^y \) on \( y \). Targeted at this, the proof is structured in the following manner. First, Lem. [3] shows that the induced measure \( \pi^V \) on configuration space continuously depends on the potential \( V \), based on which Cor. [4] ensures that the thermal average \( G^A (V) \) is a continuous with respect to \( V \). Then Lem. [5] shows that the induced measure \( \mu^y \) on potential space continuously depends on the training observation \( y \). The main theorem (Thm. [6]) utilizes the two lemmas and the
formula for \( \pi^y \) to control the perturbation between \( \pi^y \) by that between \( \mu^y \), leading to the conclusion. Finally, Cor. 7 shows how to bound the perturbation in testing observations by that in training observations.

**Notation.** Given a separable Banach space \( \mathcal{X} \) and two functions \( f_1, f_2 \) on \( \mathcal{X} \times \mathcal{X} \). We call \( f_1 \succ_r f_2 \) if, for every fixed \( r > 0 \), there is \( C = C(r) > 0 \) such that

\[
f_1(x,x') \leq Cf_2(x,x'), \forall x, x' \in B_\mathcal{X}(0,r).
\]

**Lemma 3.** Given two potential functions \( V_1, V_2 \in W^1 \), we have

\[
d_{\text{Hell}}(\pi^{V_1}, \pi^{V_2}) \lesssim_r \|V_1 - V_2\|_{W^1}
\]

where the definition of Hellinger distance is given by Def. 14 in the Appendix.

The proof of this lemma is a direct application of Thm. 18 in the Appendix.

**Proof.** First we check the conditions for Assu. 17: notice that \( \Phi(q; V) = \int_0^\beta \hat{V} \circ q \, d\tau \) is continuous as a function of \( q \), and that

\[
|\Phi(q; V_1) - \Phi(q; V_2)| = \left| \int_0^\beta (V_1 - V_2) \circ q \, d\tau \right| \leq \beta \|V_1 - V_2\|_\infty \leq \beta \|V_1 - V_2\|_{W^1},
\]

thus we can take \( M_1(r) = \beta r \) and \( M_2 = \beta \).

Since \( M_1 \) and \( M_2 \) are constant with respect to \( q \), by Thm. 18 there exists \( C = C(r) \) such that for all \( V_1, V_2 \in B_{W^1}(0,r) \),

\[
d_{\text{Hell}}(\pi^{V_1}, \pi^{V_2}) \leq C \|V_1 - V_2\|_{W^1}.
\]

**Corollary 4.** The ensemble average of a given bounded observable \( A \) is continuous as a function of the potential function, i.e.

\[
|G^A(V_1) - G^A(V_2)| \lesssim_r \|V_1 - V_2\|_{W^1}
\]

where \( G^A(V) \triangleq \mathbb{E}_{\pi^V(dq)} \frac{1}{\beta} \int_0^\beta A \circ q \, d\tau = \mathbb{E}_{\pi^V(dq)} A[q] \).

**Proof.** This is a direct corollary of Lem. 19 and Lem. 3 since \( G^A(V) \) is a bounded function on \( W^1 \).

**Lemma 5.** Given two training observations \( y_1, y_2 \) and assume the training observable \( A \) is bounded, we have

\[
d_{\text{Hell}}(\mu^{y_1}, \mu^{y_2}) \lesssim_r \|y_1 - y_2\|_2
\]

where \( \|\cdot\|_2 \) is the Euclidean norm on \( \mathbb{R}^{NT} \) and the Hellinger distance is given by Def. 14.

The proof of this lemma is another direct application of Thm. 18.
Proof. Again we check the conditions for Assu. [7], notice that

\[
\Phi (V; y) = \frac{1}{2} \left\| \Gamma^{-\frac{1}{2}}_\eta \left( y - G^A (V) \right) \right\|_2^2 - \frac{1}{2} \left\| \Gamma^{-\frac{1}{2}} \eta y \right\|_2^2
\]

is continuous as a function of the two variables \((V, y)\) (by Cor. [4]), and that

\[
\Phi (V; y) \geq - \frac{1}{2} \left\| \Gamma^{-\frac{1}{2}} \eta y \right\|_2^2,
\]

\[
|\Phi (V; y_1) - \Phi (V; y_2)| \leq \left[ \frac{1}{2} \| y_1 + y_2 \|_2 + \| A \|_\infty \right] \| \Gamma^{-1}_\eta \|_2 \| y_1 - y_2 \|_2,
\]

we can take \(M_1 = \frac{1}{2} \| \Gamma^{-\frac{1}{2}} \eta y \|_2^2\) and \(M_2 (r) = \| \Gamma^{-1}_\eta \|_2 (r + \| A \|_\infty)\), where \(\| \Gamma^{-1}_\eta \|_2\) is the operator norm induced by the vector norm \(\| \cdot \|_2\). Since they are also constant with respect to \(V\), by Thm. [18] there is \(C = C (r)\) such that for all \(y_1, y_2 \in By (0, r)\),

\[
d_{Hell} (\mu^{y_1}, \mu^{y_2}) \leq C \| y_1 - y_2 \|_2. \tag*{\Box}
\]

**Theorem 6.** Given two training observations \(y_1, y_2\) and assume the training observable \(A\) is bounded, the distance between two induced measure on \(\mathcal{L}^2\) can be bounded by the their distance, i.e.

\[
d_{TV} (\pi^{y_1}, \pi^{y_2}) \leq_r \| y_1 - y_2 \|_2.
\]

**Proof.** The proof consists of two steps: first we will bound the distance between \(\pi^y\) by the distance between \(\mu^y\), then we will compare the latter part with the distance between \(y\).

By definition of TV distance and the fact that \(\pi^y \ll \pi_0\), we can expand the left-hand side as

\[
d_{TV} (\pi^{y_1}, \pi^{y_2}) = \int_{\mathcal{L}^2} \pi_0 (dq) \left| \frac{d\pi_{y_1}}{d\pi_0} (q) - \frac{d\pi_{y_2}}{d\pi_0} (q) \right|
\]

\[
= \int_{\mathcal{L}^2} \pi_0 (dq) \left| \int_{W^1} \mu_0 (dV) \frac{d\pi_V}{d\pi_0} (q) \left[ \frac{d\mu_{y_1}}{d\mu_0} (V) - \frac{d\mu_{y_2}}{d\mu_0} (V) \right] \right|
\]

where the second equation results from the definition of \(\pi^y\) (Eqn. [19]). By taking the absolute sign into the second integral and a change to the order of integral (by Tonelli’s theorem), we have

\[
d_{TV} (\pi^{y_1}, \pi^{y_2}) \leq \int_{\mathcal{L}^2} \pi_0 (dq) \left[ \int_{W^1} \mu_0 (dV) \frac{d\pi_V}{d\pi_0} (q) \left| \frac{d\mu_{y_1}}{d\mu_0} (V) - \frac{d\mu_{y_2}}{d\mu_0} (V) \right| \right]
\]

= \int_{W^1} \mu_0 (dV) \left[ \int_{\mathcal{L}^2} \pi_0 (dq) \frac{d\pi_V}{d\pi_0} (q) \left| \frac{d\mu_{y_1}}{d\mu_0} (V) - \frac{d\mu_{y_2}}{d\mu_0} (V) \right| \right].

Notice that the R-N derivative \(\frac{d\mu^y}{d\mu_0} (V)\) does not depend on \(q\), we can take the term outside the second integral:

\[
d_{TV} (\pi^{y_1}, \pi^{y_2}) \leq \int_{W^1} \left\{ \mu_0 (dV) \left| \frac{d\mu_{y_1}}{d\mu_0} (V) - \frac{d\mu_{y_2}}{d\mu_0} (V) \right| \left[ \int_{\mathcal{L}^2} \pi_0 (dq) \frac{d\pi_V}{d\pi_0} (q) \right] \right\}.
\]
Now we can directly calculate the second integral since \( \int_{\mathcal{L}} \pi_0 \left( dq \right) \frac{d\pi}{d\pi_0} \left( q \right) = \int_{\mathcal{L}} \pi \left( dq \right) = 1 \), so again by the definition of TV distance

\[
d_{TV} \left( \pi_{y_1}, \pi_{y_2} \right) \leq \int_{W_1} \mu_0 \left( dV \right) \left| \frac{d\mu_{y_1}}{d\mu_0} \left( V \right) - \frac{d\mu_{y_2}}{d\mu_0} \left( V \right) \right|
\]

By Lem. \( \text{[15]} \) we can bound the TV distance by the Hellinger distance, leading to

\[
d_{TV} \left( \pi_{y_1}, \pi_{y_2} \right) \leq d_{TV} \left( \mu_{y_1}, \mu_{y_2} \right) \leq \sqrt{2} d_{\text{Hell}} \left( \mu_{y_1}, \mu_{y_2} \right) \lesssim r \| y_1 - y_2 \|_2,
\]

where the second inequality holds as a result of Lem. \( \text{[6]} \).

**Corollary 7.** Given two training observations \( y_1, y_2 \) and assume the training and testing observables \( A, O \) are bounded, the difference between the expectations of the testing observable w.r.t the two posterior distributions can be bounded by the distance of training observations:

\[
\left| \mathbb{E}_{\pi_{y_1}} O \left( q \right) - \mathbb{E}_{\pi_{y_2}} O \left( q \right) \right| \lesssim r \| y_1 - y_2 \|_2.
\]

**Proof.** This is a direct corollary of Lem. \( \text{[19]} \) and Thm. \( \text{[6]} \) since \( O \left( q \right) = \frac{1}{\beta} \int_0^\beta O \left( q \left( \tau \right) \right) d\tau \) is a bounded function on \( \mathcal{X} \).

**Remark.** We shall revisit this corollary on stability in the numerical study section.

6 Numerical tests (1 level system)

6.1 Proof of concept

First we will demonstrate that the algorithm works in a one-dimensional system setting if the training observation \( y^* \) is assumed without noise. The system is set-up as follows:

- Ground-truth potential function \( V_{\text{truth}} = \frac{1}{2} x^2 + 5 \sin \left( \frac{5x}{\pi} \right) \exp \left( -\frac{x^2}{2} \right) \), shown in Fig. \( \text{[1]} \)
- Training observable \( A_i = e^{-\left( x-x_i \right)}^2 \) where \( x_i = \frac{i}{2} - 2, i = 0 \ldots 8 \), i.e. a series of Gaussians along the most probable locations.
- Testing observable \( O_1 = \phi_1 \left( 2x \right), O_2 = e^{-\left( x+1.25 \right)}^2, O_3 = e^{-\left( x-0.25 \right)}^2, O_4 = \phi_2 \left( 3x \right), O_5 = \phi_3 \left( 3x \right) \).
- The noise covariance matrix \( \Gamma_\eta = \frac{1}{N_1} I_{N_1 \times N_1} \) with \( \Gamma_0 = 10^{-3} \)
- The potential covariance sequence \( \gamma_j = 4 \cdot j^{-1.2} \) \( \left( j = 0 \ldots 12 \right) \).
- Particle mass \( M = 10 \), truncation level \( L = 12 \) and bead number \( N = 16 \).
Figure 1: Left figure: the ground truth potential $V_{\text{truth}}$ (green line) is lower near $x = -1$ and higher near $x = 1$ as compared to the harmonic oscillation potential (brown faded line, also used as the initial potential $V^{(0)}$).

Top-right figure: illustration for training observables $\{A_j\}_{j=0}^8$, each of which is a Gaussian function distributed along the most probable locations.

Bottom-right figure: illustration for testing observables $\{O_j\}_{j=1}^5$, varying in the size of support set and oscillation intensity. Among the five testing observables, the first two will be selected for demonstration since the rest three give similar results.

We ran 10 independent runs in total with 400 proposals in each run. We select two of the five testing observables to report since the results of the rest three are similar. In the following figures, we will always label the initial guess (obtained at the first iteration, i.e. by setting the harmonic oscillation potential $V_o = \frac{1}{2}x^2$) as the brown dotted line and the ground truth (obtained by setting ground truth $V_{\text{truth}}$) as the green dashed line; we also indicate twice the standard error by the shaded area.

The results are shown in Fig. 2 and 3. Judging from the figures, the potential and density landscapes can correctly sampled where the probability density is relatively large. As for the thermal average of the testing observables, the averaged samples will converge towards the ground truth and the standard error will decrease over iterations. We will further discuss the residual between the convergent value and the ground truth in the following sections.

### 6.2 Stability result: A numerical proof

Recall the form of theorem on stability (Cor. 7):

$$\left| \mathbb{E}_{\pi_{y_1}} O[q] - \mathbb{E}_{\pi_{y_2}} O[q] \right| \lesssim \gamma \|y_1 - y_2\|_2 ,$$

this inequality describes how the perturbation of output testing observations are bounded by that of the input training observations. To be more specific, we can interpret it in the following two ways:

1. Given noise covariance matrix $\Gamma_\eta$, the theorem ensures that the output predictions should rely on the input training observations continuously, thus leading to a stable numerical algorithm.
Figure 2: Sampled test observations averaged along the proposal-decision iterations. In each of the two figures, the blue/red line corresponds to the averaged samples for the 1st/2nd test observable. The shaded area indicates twice the standard error with respect to different independent runs. The green line stands for the ground-truth thermal average of the test observable. The faded brown line stands for the value sampled at the initial iteration by setting the potential \( V \) to be the harmonic oscillation potential \( V_o \).

Figure 3: Averaged sampled potential functions \( \frac{1}{K_{\text{total}}} \sum_{k=1}^{K_{\text{total}}} V^{(k)} \) (left figure) and density functions (right figure). Shaded area indicates twice the standard error with respect to different independent runs. Green dashed line: obtained by setting the potential of the system to the ground-truth potential \( V_{\text{truth}} \). Faded brown line: obtained from the harmonic oscillation potential \( V_o \) (also used as the initial condition \( V^{(0)} \)).

2. More generally, the theorem also describes how consistent the output predictions on test observables are if the noise covariance is specified. Consider the following formal deduction. Let \( y^* \) be the thermal average of training observables and \( V_{\text{truth}} \) be the potential function. The distribution of the noisy training observation \( y \) is \( \mathcal{N}(y^*, \Gamma_\eta) \), merely a translation of the distribution of the noise \( \eta \). According to Jensen’s inequality, the expectation of the input disturbance can be estimated by interchanging the expectation operator and the quadratic function:

\[
E_{y \sim \mathcal{N}(y^*, \Gamma_\eta)} \|y - y^*\|_2 \leq \sqrt{E_{\mathcal{N}(0, \Gamma_\eta)} \|\eta\|_2^2} = \sqrt{\text{Tr}(\Gamma_\eta)}.
\]
On the other hand, when $Tr(\Gamma_\eta)$ is small enough, the measure $\mu_{y^*}$ induced on the potential space $W^1$ will converge to the delta measure $\delta(V - V_{truth})$, so the test prediction $E_{q \sim \pi_{y^*} O}[q]$ should converge to $G^O(V_{truth})$, i.e. the ground-truth thermal average of test observables. To sum up, if we draw a few training observations from $N(y^*, \Gamma_\eta)$ and send them through the inversion process, the error in output test predictions compared to the ground truth can be estimated by the following inequality

$$error = E_{y \sim N(y^*, \Gamma_\eta)} \left| E_{q \sim \pi_y O}[q] - G^O(V_{truth}) \right| \lesssim \sqrt{Tr(\Gamma_\eta)}.$$ (22)

In the following experiments, we will assume different scales for the noise covariance and compare the corresponding test observations. As in the previous section, the noise covariance is set to $\Gamma_\eta = \tilde{\Gamma}_\eta I_{N_1 \times N_1}$, where $\tilde{\Gamma}_\eta = 0.01, 0.03, 0.1, 0.3$.

![Figure 4: Testing observations compared among experiments if different scales of noise covariance $\tilde{\Gamma}_\eta$ are assumed. Horizontal axis: the scale of noise variance $\tilde{\Gamma}_\eta$. Vertical axis: test observations, where the green dashed line stands for the ground truth. The solid bars stand for the mean and standard error of test observations (faded dots) obtained in numerical experiments.](image)

Judging from Fig. 4, we can see that a smaller $\tilde{\Gamma}_\eta$ will lead to a more accurate mean and a smaller variance of the sampled test observations. Furthermore, if we fit the error with the scale of noise covariance $\tilde{\Gamma}_\eta = \frac{1}{N_T} Tr(\Gamma_\eta)$ ($N_T$ is the fixed number of training observables), the slope in log scale (see Fig. 5) is around $\frac{1}{2}$, which is consistent with Eqn. 22.

### 6.3 Numerical study on 2-Level system

#### 6.3.1 Problem formulation

In the previous sections, we have build a rigorous theory on Bayesian inversion in the quantum thermal average problem. It is tempting to extend this theory into a broader area where the quantum system is associated with multiple electronic states and non-adiabatic effects are taken into account. Under a few technical assumptions, the extension can be quite straightforward since the essential procedures are kept the same: the potential function can induce a probability measure on the bead configuration space, while the thermal average can be compared to the ground truth of training observations to induce a probability measure on the potential function space. The prime difficulty lies in the forward
Figure 5: Log scale figure for test observation errors and noise covariance scales $\tilde{\Gamma}_\eta$, indicating that assuming smaller noise covariances can lead to more consistent test observations sampled. Color folded line: averaged test observation errors obtained from numerical experiments. Grey dashed line: reference line with slope $\frac{1}{2}$. The fitted slopes for two folded lines are listed in the legend.

problem of finding an efficient way to sample the distribution on the bead configuration space, which is concerned in [Lu and Zhou, 2017] and PIMD-SH is thus developed. We refer to Sec. B in the Appendix for details. In the following sections we will basically transfer the algorithm proposed for 1-level systems to 2-level systems and demonstrate corresponding numerical studies.

6.3.2 Notations

The space of 2-level potential functions $V$ is defined as

$$W^2 \triangleq \left\{ V = \begin{pmatrix} V_{00} & V_{01} \\ V_{01} & V_{11} \end{pmatrix} : V_{00}, V_{11} \in W^1, V_{01} \in W^g \right\}$$

and $W^g$ denotes the following mixed-Gaussian-component space

$$W^g \triangleq \left\{ V_{01} : V_{01}(x) = \sum_{i=1}^{N_{\text{off}}} A_i \exp \left( -\frac{(x - c_i)^2}{2\sigma_i^2} \right) \right\}$$

where we have the following assumptions:

- the off-diagonal potential component number $N_{\text{off}}$, location series $\{c_i\}$ and derivation series $\{\sigma_i\}$ are known and fixed,
- each amplitude component $A_i \in \mathbb{R}^+$ is unknown.

6.3.3 Algorithm explanation

There are two main differences compared from the 1-level algorithm (Alg. 1):

1. The proposal of $V$: since we are now dealing with $V \in W^2$, not only the diagonal terms $V_{00}$ and $V_{11}$ are sampled as in the 1-level case, but also the off-diagonal term should be sampled. The prior for $V_{01}$ (essentially for $\{A_i\}$ since the other parameters are fixed) is chosen as the exponential distribution, which can be efficiently proposed by Alg. 3.
2. The sampling of \((q,l)\): it is accomplished by the implementation of PIMD-SH. We refer to Sec. \[2\] in the Appendix for details.

### 6.3.4 Numerical study set-up

Here we conduct tests for the following system:

\[
\begin{align*}
V_{00} &= \frac{1}{2}x^2 - \frac{3}{2}\phi_1(x) \\
V_{01} &= \exp(-2x^2) \\
V_{11} &= \frac{1}{2}x^2 - \frac{3}{4}\phi_0(x) - \frac{3}{2}\phi_1(x) - \phi_2(x)
\end{align*}
\]

where the off-diagonal potential has \(N_{\text{off}} = 1\) Gaussian component and \(A_1 = 1\) (unknown and to be recovered), \(\sigma_1 = 0.5, c_1 = 0\) (fixed and known beforehand). The two diagonal-potentials almost intersect near \(x = 0\), where \(V_{01}\) is significantly positive, providing chances for hopping between layers. Besides, the particle mass \(M\) is set to 10, truncation level \(L\) to 4 and bead number \(N\) to 8.

The observables we used in training/testing have either diagonal or off-diagonal non-zero entries only. For those only with diagonal entries, we simply set the two diagonal entry to be the same, while those only with off-diagonal entries have the same off-diagonal real-valued entries since the observables are Hermite. The training observables have diagonal Gaussian entries in between \([-2, 2]\) and off-diagonal Gaussian entries in between \([-1, 1]\). The testing observables are

\[
\begin{align*}
O_1 &= \begin{pmatrix} o_1 \\ o_1 \end{pmatrix}, \quad o_1 = \exp\left(-\frac{(x-1.25)^2}{4}\right) \\
O_2 &= \begin{pmatrix} o_2 \\ o_2 \end{pmatrix}, \quad o_2 = \exp\left(-\frac{(x+0.25)^2}{4}\right) \\
O_3 &= \begin{pmatrix} o_3 \\ o_3 \end{pmatrix}, \quad o_3 = \exp\left(-8(x - 0.1)^2\right) \\
O_4 &= \begin{pmatrix} o_4 \\ o_4 \end{pmatrix}, \quad o_4 = \exp\left(-8(x - 0.3)^2\right)
\end{align*}
\]

as shown in Fig 6.

### 6.3.5 Numerical results and discussions

Likewise, we demonstrate that the algorithm in the 2-level setting can recover potential landscape and predict test observables. As shown in Fig. 7 and 8, the sampled average will start from the initial value (marked by the brown line) and converge to the proposed average \(\mathbb{E}_{\pi_y}O(q)\), which is quite close to the ground truth (marked by the green line). The potential learned exhibits a tendency to be deeper near \(x = 1\), which captures the landscape of ground truth potentials.

In a non-adiabatic system, it is quite reasonable to speculate that training with off-diagonal-only observables (i.e. vanish along the diagonal line and only having off-diagonal terms) will help recover the potential landscape more accurately. Fig. 9 shows the comparison between results obtained by
Figure 6: Illustration on ground-truth potential (left-most) and training (middle)/testing (right-most) observables in 2-level system. Top rows show observables with only diagonal entries and bottoms rows show observables with only off-diagonal entries.

Figure 7: Observations for test observables averaged along the proposal-decision iterations. Top two figures: diagonal-only testing observables $\hat{O}_1$ (teal), $\hat{O}_2$ (light blue). Bottom two figures: off-diagonal-only testing observables $\hat{O}_3$ (red), $\hat{O}_4$ (orange). Green solid line: ground truth. Faded brown dashed line: a guess based on the initial potential function.

training the system with and without off-diagonal-only observables. It is especially clear that the ‘with’ condition outperforms in the off-diagonal-only test observables in terms of convergence speed and bias.
8 Conclusion

In this paper, we proposed a novel method regarding the inversion problem of quantum thermal average. By adopting the Bayesian inversion framework, we not only obtain a posterior distribution of potential functions based on finite noisy observations, but also the stability result is established under the framework and the numerical algorithm is proved to be efficient. In the numerical section, we have shown that the ensemble average of bounded testing observables can be accurately sampled, and furthermore the error can be controlled by the assumed perturbation in the input training data, which testifies our theoretical result (Thm. 6). We also demonstrated how to apply the algorithm to the non-adiabatic regime. Since the tests in the 2-level setting are preliminary and the accuracy is not satisfactory, it indeed requires more attention and effort on the improvement. In addition, it is not clear yet what observables are favorable in order to have a consistent approximation of the potential function.

Here we ought to mention that this work can easily extend to related problems. First, our method can be extended to systems in higher dimensions. One can easily verify that Thm. 6 still holds...
if the loop space \( X \) is extended to \( \mathbb{L} \mathbb{R}^d \) and potential space \( W^1 \) is modified accordingly. As for the numerical implementation, we can expand the potential onto tensor product of Hermite basis. Second, judging from the numerical Sec5.3 our method fits multi-level systems quite well. A similar theoretical stability result can also be obtained if the Boltzmann distribution follows the form in the single-level system. Future investigations on a more general function space \( W^g \) setting for the off-diagonal potential functions may yield better results. At the same time, the framework proposed in this work is compatible with all kinds of solvers for the forward problem, so the methods developed in \([\text{Liu and Liu, 2018}]\) \([\text{Lu and Zhou, 2018a}]\) \([\text{Tao et al., 2018}]\) can be seamlessly integrated into the algorithm. Besides, if given multiple training observations, we can also make use of the Ensemble Kalman Filter (EnKF) \([\text{Mandel, 2009}]\) to improve the accuracy.

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A Analysis Supplements

**Lemma 8.** The vector space $W \triangleq L^2(\mathbb{R}) \cap L^\infty(\mathbb{R})$ is a Banach space under the norm

$$
||f||_W \triangleq ||f||_{L^2(\mathbb{R})} + ||f||_{L^\infty(\mathbb{R})}.
$$

**Proof.** It suffices to show that a Cauchy sequence $\{f_n\}$ in $W$ converges in $W$. In fact, $\{f_n\}$ is also a Cauchy sequence in $L^2(\mathbb{R})$ and in $L^\infty(\mathbb{R})$. Denote the corresponding limit as $f_n \xrightarrow{L^2(\mathbb{R})} h$ and $f_n \xrightarrow{L^\infty(\mathbb{R})} \overline{h}$.

Restricted on a given interval $[a, b]$, notice that $||\cdot||_{L^2([a, b])} \leq ||\cdot||_{L^2(\mathbb{R})}$ and $||\cdot||_{L^\infty([a, b])} \leq ||\cdot||_{L^\infty(\mathbb{R})}$, we have $h \in L^2([a, b])$ and $\overline{h} \in L^\infty([a, b])$. However, for $g_n \triangleq f_n - \overline{h} \in L^\infty([a, b])$,

$$
||g_n||_{L^2([a, b])} \leq \sqrt{(b-a)} ||g_n||_{L^\infty([a, b])} \leq \sqrt{b-a} ||g_n||_{L^\infty([a, b])},
$$

so $g_n$ converges to 0 in $L^2([a, b])$, i.e. $f_n \xrightarrow{L^2([a, b])} \overline{h}$. But $f_n$ also converges to $h$ in $L^2([a, b])$, so $h$ and $\overline{h}$ a.e. agree with each other on $[a, b]$.  

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Then, since \( h \) and \( \hat{h} \) a.e. agree on \([-N,N]\), they a.e. agree on \( \mathbb{R} \), so \( f_n \) converges to \( h \in L^2(\mathbb{R}) \cap L^\infty(\mathbb{R}) \) under the \( ||\cdot||_W \) norm.

\[\Box\]

**Definition 9.** The Hermite function sequence \( \{\phi_n\} \) is defined as

\[
\phi_n(x) \triangleq (-1)^n (2^n n! \sqrt{\pi})^{-\frac{1}{2}} e^{-x^2} \frac{d^n}{dx^n} e^{-x^2}.
\]

**Theorem 10.** Let \( D \subset \mathbb{R}^d \) be a compact domain, \( \{\gamma_k\}_{k \geq 0} \) be a real-valued sequence and \( \{\xi_k\}_{k \geq 0} \) be countably many centered i.i.d. random variables with bounded moments of all orders. Assume that \( \{\psi_k\}_{k \geq 0} \) is a sequence of Hölder functions satisfying

\[
|\psi_k(x)| \leq C_1, \quad \forall k \geq 0, x \in D
\]

\[
|\psi_k(x) - \psi_k(y)| \leq C_2 k^{\alpha} |x - y|^{\alpha}, \quad \forall k \geq 0, x \in D
\]

where \( C_1, C_2 \) are constants and \( \alpha \in (0,1], t > 0 \). Suppose there is some \( \delta \in (0,2) \) such that

\[
S_1 \triangleq \sum_{k \geq 0} \gamma_k^2 < \infty \quad \text{and} \quad S_2 \triangleq \sum_{k \geq 0} \gamma_k^{2 - \delta} k^{\delta} < \infty.
\]

Then \( u \) defined by

\[
u \triangleq \sum_{k \geq 0} \gamma_k \xi_k \psi_k
\]

is a.s. finite for every \( x \in D \), and \( u \in C^{0,\alpha'}(D) \) for every \( \alpha' < \alpha \delta/2 \) (i.e. \( u \) is Hölder continuous for every exponent smaller than \( \alpha \delta/2 \)).

This theorem is a direct corollary which can be found in [Dash and Stuart, 2017], Page 91.

**Proposition 11.** Assume the positive sequence \( \gamma_j = O(j^{-s}) \) with \( s > 1 \) and \( \{\xi_j\}_{j=1}^\infty \) are i.i.d. random variables with finite second moment. Denote the Hermite functions as \( \{\phi_n\} \) defined in 9. Then the function series \( \sum_{j=0}^\infty \xi_j \gamma_j \phi_j \) \( \mathbb{P} \)-a.s. converges in \( W^1 = L^\infty \cap L^2 \) with norm \( ||\cdot||_{W^1} = ||\cdot||_{L^2} + ||\cdot||_{L^\infty} \).

**Proof.** We will use the following lemma without proof: let \( \{I_j\}_{j=0}^\infty \) be a sequence of \( \mathbb{R}^+ \)-valued independent random variables, then the following equivalence holds:

\[
\sum_{j=0}^\infty I_j < +\infty \mathbb{P}\text{-a.s.} \iff \sum_{j=0}^\infty \mathbb{E}(I_j \wedge 1) < \infty.
\]

For the \( L^\infty \) part, we denote \( I_j^{(1)} = ||\xi_j \gamma_j \phi_j||_{L^\infty} \). By Cramér’s inequality \( ||\phi_n||_{L^\infty} \leq \pi^{-\frac{1}{2}} \), we have

\[
\sum_{j=0}^\infty \mathbb{E}I_j^{(1)} = \sum_{j=0}^\infty \gamma_j ||\phi_j||_{L^\infty} \mathbb{E} |\xi_j| \leq \pi^{-\frac{1}{2}} \sum_{j=0}^\infty \gamma_j.
\]
For the $L^2$ part, we denote $I_j^{(2)} = ||\xi_j \gamma_j \phi_j||_{L^2}$, then

$$\sum_{j=0}^{\infty} E I_j^{(2)} = E |\xi_j| \sum_{j=0}^{\infty} \gamma_j$$

Since we already assumed that $\gamma_j = O(j^{-s})$ with $s > 1$, the infinite sums $\sum_{j=0}^{\infty} \gamma_j$ and $\sum_{j=0}^{\infty} \gamma_j^2$ are finite, so

$$\sum_{j=0}^{\infty} E (||\xi_j \gamma_j \phi_j||_{W^1} \wedge 1) \leq \sum_{j=0}^{\infty} E I_j^{(1)} + \sum_{j=0}^{\infty} E I_j^{(2)}$$

$$\leq \left(1 + \pi^{-\frac{1}{4}}\right) E |\xi_j| \sum_{j=0}^{\infty} \gamma_j$$

$$< \infty.$$

According to the lemma we stated at the beginning of the proof, the infinite sum $\sum_{i=0}^{\infty} ||\xi_i \gamma_i \phi_i||_{W^1}$ P.a.s. converges. By the completeness of $W^1$, the function series $\sum_{i=0}^{\infty} \xi_i \gamma_i \phi_i$ P.a.s. converges to a $W^1$ function.

**Proposition 12.** Assume the positive sequence $\gamma_j = O(j^{-s})$ with $s > \frac{1}{2}$ and $\xi_j \sim N(0,1)$. Denote the Hermite functions defined in [9] as $\{\phi_n\}$. Then for all $\beta < \frac{4s-2}{4s+1}$, the function series $\sum_{j=0}^{\infty} \xi_j \gamma_j \phi_j$ P.a.s. converges in $C^{0,\beta}(\mathbb{R})$.

**Proof.** First we fix the domain $D_R$ restricted to $[-R,R]$. By Thm. 10, the series of interest has proper regularity as long as $S_1$ and $S_2$ are finite. The key of this proof is to identify constants $t$ and $\alpha$ satisfying

$$|\phi_n(x) - \phi_n(y)| \leq C_2 n^t |x-y|^\alpha$$

for any $x, y \in D_R$ and $n \in \mathbb{N}$.

For Hermite basis functions, $\arg \max |\phi'_n| = 0$ if $n$ is odd. If we take $p = \frac{n+1}{2}$, we can have the following equation after some tedious calculations:

$$|\phi'_n(0)| = \frac{\sqrt{(2p-1)!}}{2^{p-1} (2\pi)^{\frac{p}{2}} (p-1)!}.$$ 

By Stirling formula,

$$\log |\phi'_n(0)| = \frac{1}{4} \log (n+1) - \frac{1}{2} \log \pi - \frac{1}{8(n+1)} + O(n^{-2}),$$

which indicates that $t = \frac{1}{4}$.

By assumption, $\gamma_j = O(j^{-s})$, we have

$$S_1 < \infty \iff s > \frac{1}{2},$$

$$S_2 < \infty \iff -(2 - \delta) s + t \delta < -1 \iff \delta < \frac{2s - 1}{s + t} = \frac{8s - 4}{4s + 1}.$$
So by Thm. 10, the function series \( \sum_{j=0}^{\infty} \xi_j \gamma_j \phi_j \) is Hölder continuous on \( D_R \) for every exponent smaller than \( \frac{4s-2}{4s+1} \). Since \( \mathbb{R} = \bigcup_{R=1}^{\infty} D_R \) and the Hölder continuity of the function series \( \mathbb{P} \)-a.s. holds for countably many \( R \), it also \( \mathbb{P} \)-a.s. holds on \( \mathbb{R} \).

## B  RPR in Two-level Systems

### B.1 Ring polymer representation

Without loss of generality, a few assumptions have been made in [Lu and Zhou, 2017]:

1. The total level of energy in the system is 2.

2. The potential function \( V = \left( \begin{array}{cc} V_{00} & V_{01} \\ V_{01} & V_{11} \end{array} \right) \) is Hermite and the off-diagonal term \( V_{01} \) keeps its sign.

3. The observable \( \hat{A} \) only depends on position \( q \).

To fully describe the bead, a level index vector \( l \in \{0, 1\}^N \) is needed besides the position configuration \( q \in \mathbb{R}^N \). By a similar induction and introduction of auxiliary momentum variable \( p \) as in the single level system, we arrive at the following formula for the thermal average

\[
\langle \hat{A} \rangle = \frac{1}{Z_N} \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} \sum_{l \in \{0, 1\}^N} W_N[A] e^{-\beta_N H_N(q, p, l)} dq dp + \mathcal{O}(N^{-2}),
\]

where the weight function is given by

\[
W_N[A](q, p, l) \triangleq \frac{1}{N} \sum_{k=1}^{N} \left( \langle l_k | A(q_k) | l_k \rangle - \text{sgn} \left( V_{l_k, l_k} \right) \langle l_k | A(q_k) | l_k \rangle \exp \left[ \beta_N \left( \langle l_k | G_k | l_{k+1} \rangle - \langle l_k | G_k | l_{k+1} \rangle \right) \right] \right),
\]

the Hamiltonian given by

\[
H_N(q, p, l) = \sum_{k=1}^{N} \langle l_k | G_k | l_{k+1} \rangle,
\]

the matrix \( G_k \) given by

\[
\langle l | G_k | l' \rangle = \begin{cases} \frac{p^2}{2M} + \frac{M(q_k - q_{k+1})^2}{2\beta_N^2} + V_{ll}(q_k) - \frac{1}{\beta_N} \log \left( \cosh \left( \beta_N |V_{01}(q_k)| \right) \right) & l = l' \\ \frac{p^2}{2M} + \frac{M(q_k - q_{k+1})^2}{2\beta_N^2} + V_{ll}(q_k) + V_{11}(q_k) - \frac{1}{\beta_N} \log \left( \sinh \left( \beta_N |V_{01}(q_k)| \right) \right) & l \neq l' \end{cases},
\]

shorthand notation \( \overline{l_i} = 1 - l_i \) and \( Z_N \triangleq \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} \sum_{l \in \{0, 1\}^N} \exp \left[ -\beta_N H_N(q, p, l) \right] dq dp \) the normalization constant.

### B.2 PIMD-SH: An abstract

The central idea of PIMD-SH is to construct a reversible Markov process that the invariant distribution is exactly \( \frac{1}{Z_N} \exp \left( -\beta_N H_N(q, p, l) \right) \). To achieve this, the dynamics of the position and momentum
variable \( z \triangleq (q, p) \) is similar to Eqn. \( 9 \) as

\[
\begin{align*}
\frac{dq}{dt} &= \nabla_p H_N (q(t), p(t), l(t)) dt \\
\frac{dp}{dt} &= -\nabla_q H_N (q(t), p(t), l(t)) dt - \gamma p dt + \sqrt{\frac{2M}{\beta_N}} dB.
\end{align*}
\]

(30)

The evolution of \( l(t) \) follows a surface hopping type dynamics, essentially a Q-process: for given index configuration \( l \), we restrict that the post-changing state can only be \( l \) or those \( l' \) which has distance 1 to \( l \). The hopping intensity from \( l \) to other possible states is determined by the following detailed balance condition

\[
p_{l',l}(z) \exp \left[ -\beta_N H_N (z, l) \right] = p_{l,l'}(z) \exp \left[ -\beta_N H_N (z, l') \right]
\]

up to an overall scaling parameter \( \eta \).

In [Lu and Zhou, 2017] the choice for \( p_{l',l}(z) \) was \( \exp \left[ \frac{\beta_N}{2} (H_N (z, l) - H_N (z, l')) \right] \), which is not upper-bounded, causing numerical difficulties if the overall hopping probability exceeds 1. Hence, in this article we propose the Hastings-style transition intensity \( \min \left\{ 1, \exp \left[ \frac{\beta_N}{2} (H_N (z, l) - H_N (z, l')) \right] \right\} \).

Once the theory for dynamics is fully established, we can apply the theorem of ergodicity

\[
\langle \hat{A} \rangle = \lim_{T \to \infty} \frac{1}{T} \int_0^T W_N [A] (\tilde{z}(t)) dt
\]

and calculate the thermal average by truncating the formula above with a finite time span.

C Bayesian Inversion Supplements

C.1 Distance between measures

Definition 13. The total variation distance between two measures \( \mu \) and \( \mu' \) is

\[
d_{TV} (\mu, \mu') \triangleq \frac{1}{2} \int \left| \frac{d\mu}{dv} - \frac{d\mu'}{dv} \right| dv.
\]

Definition 14. The Hellinger distance between \( \mu \) and \( \mu' \) is

\[
d_{Hell} (\mu, \mu') \triangleq \sqrt{\frac{1}{2} \int \left( \sqrt{\frac{d\mu}{dv}} - \sqrt{\frac{d\mu'}{dv}} \right)^2 dv}.
\]

Lemma 15. The total variation metric and the Hellinger metric are related by the following inequalities

\[
\frac{1}{\sqrt{2}} d_{TV} (\mu, \mu') \leq d_{Hell} (\mu, \mu') \leq d_{TV} (\mu, \mu')^{\frac{3}{2}}.
\]

C.2 Theorem on conditional variables

Theorem 16. Let \( (X, A) \) and \( (Y, B) \) denote a pair of measurable spaces and let \( \nu \) and \( \pi \) be probability measures on \( X \times Y \). We assume that \( \nu \ll \pi \). Thus there exists \( \pi \)-measurable \( \phi : X \times Y \to \mathbb{R} \) with
\( \phi \in \mathcal{L}_1^1 \) and
\[
\frac{d\nu}{d\pi} (x,y) = \phi (x,y).
\]
Assume that the conditional random variable \( x|y \) exists under \( \pi \) with probability distribution denoted by \( \pi^y(dx) \). Then the conditional random variable \( x|y \) exists under \( \nu \), with probability distribution denoted by \( \nu^y(dx) \). Furthermore, \( \nu^y \ll \pi^y \) and if \( c(y) \triangleq \int_X \phi (x,y) \, d\pi^y(x) > 0 \), then
\[
\frac{d\nu^y}{d\pi^y} (x) = \frac{1}{c(y)} \phi (x,y).
\]

The theorem can be found in [Dashti and Stuart, 2017], Page 28.

C.3 Well-posedness result

Notation. In this section, let \( X \) and \( Y \) be two separable Banach spaces, and \( \mu_0 \) a measure on \( X \). Given \( y \in Y \), \( \mu^y \) is defined as the measure absolutely continuous to \( \mu_0 \) by
\[
\frac{d\mu^y}{d\mu_0} (x) = \frac{1}{Z(y)} \exp \left( -\Phi(x; y) \right)
\]
\[
Z(y) = \int_X \exp \left( -\Phi(x; y) \right) \mu_0 (dx).
\]

Assumption 17. Let \( X' \) be a separable subspace of \( X \) and assume that \( \Phi \in \mathcal{C} (X' \times Y; \mathbb{R}) \). Assume further that there are functions \( M_i: \mathbb{R}^+ \times \mathbb{R}^+ \rightarrow \mathbb{R}^+ \), \( i = 1, 2 \), monotonic non-decreasing separately in each argument, and with \( M_2 \) strictly positive, such that for all \( u \in X', y, y_1, y_2 \in B_Y (0, r) \),
\[
\Phi (u; y) \geq -M_1 (r, \| u \|_X),
\]
\[
|\Phi (u; y_1) - \Phi (u; y_2)| \leq M_2 (r, \| u \|_X) \| y_1 - y_2 \|_Y.
\]

Theorem 18. Assume that Assu. 17 holds. Assume that the prior measure is a.s. restricted on the separable subspace \( X' \) (i.e. \( \mu_0 (X') = 1 \)) and that \( \mu_0 (X' \cap S) > 0 \) for some bounded set \( S \) in \( X \). Assume additionally that, for every fixed \( r > 0 \),
\[
\exp \left( M_1 (r, \| u \|_X) \right) \left( 1 + M_2 (r, \| u \|_X)^2 \right) \in \mathcal{L}_{\mu_0}^1 (X; \mathbb{R}).
\]
Then we have the following asymptotic inequality
\[
d_{Hell} (\mu^y, \mu^y') \approx_r \| y - y' \|_Y.
\]

The proof can be found in [Dashti and Stuart, 2017], Page 38-39. Thm. 18 ensures that the distance between induced posterior probability measures is bounded by the distance between different dependent variables.

Lemma 19. Given a function \( f \in \mathcal{L}_{\mu_0}^\infty (X; \mathbb{R}) \cap \mathcal{L}_{\mu_0'}^\infty (X; \mathbb{R}) \), we have
\[
\left| \mathbb{E}^{\mu^y} f (u) - \mathbb{E}^{\mu'^y} f (u) \right| \leq C (f) d_{TV} \left( \mu^y, \mu'^y \right),
\]
which leads to

\[ \left| \mathbb{E}^{\mu_y} f(u) - \mathbb{E}^{\mu_{y'}} f(u) \right| \leq r \| y - y' \|_Y \]

for fixed \( f \).

Proof. By the definition of \( d_{TV} \), there exists a measure \( \nu \) s.t. both \( \mu_y \) and \( \mu_{y'} \) are absolutely continuous w.r.t. \( \nu \); for example, take \( \nu = \frac{1}{2} (\mu_y + \mu_{y'}) \). Then a direct calculation shows that

\[
\left| \mathbb{E}^{\mu_y} f(u) - \mathbb{E}^{\mu_{y'}} f(u) \right| = \left| \int_X f \, d\mu_y(u) - \int_X f \, d\mu_{y'}(u) \right|
= \left| \int_X f \frac{d\mu_y}{d\nu}(u) - \int_X f \frac{d\mu_{y'}}{d\nu}(u) \right|
= \left| \int_X \left( \frac{d\mu_y}{d\nu} - \frac{d\mu_{y'}}{d\nu} \right) d\nu(u) \right|
\leq \| f \|_{L^\infty} \cdot \int_X \left| \frac{d\mu_y}{d\nu} - \frac{d\mu_{y'}}{d\nu} \right| d\nu(u)
= \max \left( \| f \|_{L^\infty} \| \mu_y \|_\infty, \| f \|_{L^\infty} \| \mu_{y'} \|_\infty \right) \cdot d_{TV}(\mu_y, \mu_{y'}) .
\]

The second conclusion is a direct corollary from Thm. 18 \((d_{Hell}(\mu_y, \mu_{y'}) > r \| y - y' \|_Y))\) and Lem. 15 \((d_{TV}(\mu_y, \mu_{y'}) \leq \sqrt{2} d_{Hell}(\mu_y, \mu_{y'}))\). \(\square\)

C.4 Measure preserving dynamics

The following algorithm from [Dashti and Stuart, 2017] is proposed to sample distributions in the form of \( \mu(du) = \mu_0(du) \frac{1}{Z} \exp(-\Phi) \):

**Algorithm 2** Metropolis-Hasting Algorithm Adapted to Infinite-dimensional Systems

1: Given the choice function \( a : X \times X \to [0, 1] \) and proposal kernel \( Q(u, dv) \).
2: Initialize \( k = 0 \) and first term \( u^{(0)} \in X \) in the sampling sequence.
3: while stopping criterion is not satisfied do
4: Propose \( v^{(k)} \) based on \( Q(u^{(k)}, dv) \).
5: Pick a random number \( r^{(k)} \sim U[0, 1] \), independently of \( (u^{(k)}, v^{(k)}) \).
6: if \( r^{(k)} < a(u^{(k)}, v^{(k)}) \) then
7: Accept the proposal: \( u^{(k+1)} = v^{(k)} \).
8: else
9: Reject the proposal: \( u^{(k+1)} = u^{(k)} \).
10: end if
11: end while

To preserve the desired measure, we can choose the choice function \( a \) and proposal kernel \( Q \) according to the following proposition.

**Proposition 20.** The Markov chain sampled in Alg. 2 is reversible to the measure \( \mu \sim \mu_0 \exp(-\Phi) \) if the following assumption holds: the negative log potential \( \Phi : X \to \mathbb{R} \) is upper-bounded on any bounded
set of $X$, the choice function $a(u, v) = \min \{1, \exp (\Phi (u) - \Phi (v))\}$ and the proposal kernel satisfies the reversible condition

$$\mu_0 (du) Q (u, dv) = \mu_0 (dv) Q (v, du).$$

Note. The proof is on Page 53 in [Dashti and Stuart, 2017].

D Reversible Proposals

**Gaussian distribution** For Gaussian distributions, we have the following lemma:

**Lemma 21.** Assume the prior distribution is $\mu_0 = \mathcal{N} (0, 1)$. The proposal kernel

$$Q (x, dy) \triangleq \frac{1}{\sqrt{2\pi \cdot (1 - \rho^2)}} \exp \left( -\frac{(y - \rho x)^2}{2 (1 - \rho^2)} \right) dy$$

satisfies the reversible condition in Prop. 20.

**Proof.** A direct calculation shows that

$$\mu_0 (dx) Q (x, dy) = \frac{dx \, dy}{\sqrt{2\pi \cdot (1 - \rho^2)}} \exp \left( -\frac{x^2}{2} - \frac{(y - \rho x)^2}{2 (1 - \rho^2)} \right) = \frac{dx \, dy}{\sqrt{2\pi \cdot (1 - \rho^2)}} \exp \left( -\frac{x^2}{2} + \frac{\rho xy}{1 - \rho^2} - \frac{y^2}{2} \right) = \frac{dx \, dy}{\sqrt{2\pi \cdot (1 - \rho^2)}} \exp \left( -\frac{y^2}{2} - \frac{(x - \rho y)^2}{2 (1 - \rho^2)} \right) = \mu_0 (dy) Q (y, dx).$$

Note. This is also known as the pCN(preconditioned CN) proposal [Cotter et al., 2012].

**Exponential distribution** However, no similar conclusion is found for exponential distribution yet. Nevertheless, since there is a close connection between exponential and gaussian distribution, we can propose the following algorithm:

**Algorithm 3** Local proposal kernel satisfying the reversible condition for exponential distribution.

1. Given starting value $r_0$, correlation factor $\rho \in (0, 1)$. Denote $\tilde{\rho} = \sqrt{1 - \rho^2}$.
2. Prepare two random gaussian $g_1, g_2 \sim \mathcal{N} (0, 1)$.
3. $r_n$ follows that

$$r_n = (\rho \sqrt{r_{n-1}} + \tilde{\rho} g_1)^2 + (\tilde{\rho} g_2)^2.$$

To verify that we have correctly implemented the algorithm, we examine the distribution and auto-correlation function in the Fig.[10]
Figure 10: Illustration of localized measure-preserving proposal algorithm. From top to bottom: overall distribution, trajectories, auto-correlation function.