Asymptotic convergence of the partial averaging technique

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We study the asymptotic convergence of the partial averaging method, a technique used in conjunction with the random series implementation of the Feynman-Kač formula. We prove asymptotic bounds valid for most series representations in the case when the potential has first order Sobolev derivatives. If the potential has also second order Sobolev derivatives, we prove a sharper theorem which gives the exact asymptotic behavior of the density matrices. The results are then specialized for the Wiener-Fourier series representation. It is found that the asymptotic behavior is $O(1/n^2)$ if the potential has first order Sobolev derivatives. If the potential has second order Sobolev derivatives, the convergence is shown to be $O(1/n^3)$ and we give the exact expressions for the convergence constants of the density matrices.

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I. INTRODUCTION

Path integral methods\textsuperscript{4,10} are perhaps the most important techniques utilized to account for quantum contributions in equilibrium statistical simulations for many-body systems. They are based on the Feynman-Kač formula\textsuperscript{2,3} which represents the density matrix and hence the partition function of a canonical quantum system as an infinite dimensional stochastic integral of a Brownian bridge functional.\textsuperscript{10} This stochastic integral is then approximated by a sequence of finite dimensional integrals, which in turn are evaluated by Monte Carlo techniques. The two most important families of discretization techniques, while not unrelated, can be distinguished by the way the paths are parameterized. The discrete path integral (DPI) methods\textsuperscript{4,9} utilize the Trotter product rule and appropriate short-time approximations to construct a more accurate finite-dimensional approximation of the quantum-mechanical density matrix. The random series implementations\textsuperscript{4,9} utilize the Ito-Nisio theorem\textsuperscript{10} to construct the Brownian bridge in the Feynman-Kač formula. Independent of which method is used, a major concern in the practical applications is the asymptotic rate of convergence as measured against the number of variables used to parameterize the paths $n$ as well as the computational time necessary to evaluate the various quantities involved.

The asymptotic behavior of the discrete methods is well studied\textsuperscript{7,11,12,13} and is known to be $O(1/n^2)$ if the expressions of the short-time approximations are functionals of the potential only. In contrast, the relative merits of the random series techniques are poorly understood. There are two basic implementations of the random series techniques that are important for practical applications: the partial averaging\textsuperscript{4,14} and the reweighted methods.\textsuperscript{4} In this paper, we shall study the asymptotic rates of convergence of the partial averaging method for different classes of basis entering the Ito-Nisio theorem as well as for different classes of potentials. We obtain surprisingly powerful convergence theorems and, most of the time, we provide not only the convergence order of different methods, but also the convergence constants. In the remainder of the introduction, we try to convince the reader that such an analytical study is important both theoretically and practically.

The partial averaging method has been rarely utilized in practical applications because it requires the Gaussian transform of the potential for its implementation. For real life potentials, this is a difficult but not impossible task. However, it was generally considered that the improvement the technique brings in does not warrant the effort of computing the Gaussian transform of the potential and the so-called gradient corrected partial averaging method was used instead. It has been shown that this latter method has general $O(1/n^2)$ asymptotic behavior for sufficiently smooth potentials and it has been argued that there is not much reason to suspect a better convergence rate for the full partial averaging method.\textsuperscript{4} However, more accurate numerical evidence recently presented in Ref.\textsuperscript{4} suggests that the full partial averaging method does have in fact a better behavior: if the technique is used in conjunction with the Fourier path integral approach (FPI)\textsuperscript{14,16} and if the potential is smooth enough, the asymptotic convergence is $O(1/n^3)$.

Consistent with these observations, in this paper we show that the asymptotic rate of convergence for the FPI partial averaging approximation (PA-FPI) is indeed $O(1/n^3)$ whenever the potential has second order derivatives in a sense that will be made clear in the text. While we shall prove quite general convergence results valid for almost all series representations, the PA-FPI approach, which is based on the Wiener-Fourier basis, will receive a special treatment. This is motivated by the fact that the Wiener-Fourier series representation is the optimal
The importance of the partial averaging method resides also in the fact that it acts as a prototypical strategy for improving the asymptotic rate of convergence of the random series path integral methods. As such, the reweighted random series technique achieves superior asymptotic convergence by simulating the partial averaging approach. For this reason, there is a close relation between the asymptotic rates of convergence of the two methods. While the asymptotic behavior of the reweighted method will be the object of a separate paper, we mention that such a study is greatly simplified once the convergence rates of the partial averaging method are known.

The practical importance of the convergence theorems that will be established in the present paper consists in the fact that they give a priori knowledge about the asymptotic order of convergence based only on readily verifiable properties of the potential. These theorems also provide useful estimates of the absolute error in the evaluation of the density matrices and, by integration, of the partition functions. Moreover, if the potential has second order derivatives, the estimates for the density matrix are asymptotically exact and they can be used to derive the convergence constants for many other properties, as for instance the convergence constants for the H-method and T-method energy estimators. However, such applications require careful analytical work that is beyond the scope of the present paper.

The content of the remainder of this paper is organized as follows. In the next section, we give a short review of the partial averaging method with the purpose of establishing the notation. We also provide a description of the main classes of potentials for which the asymptotic convergence will be studied. In Section III, we prove the main convergence theorems, which are valid for most series representations. We prove some asymptotic bounds for the density matrix in the case when the potential has first order Sobolev derivatives and then we give the exact asymptotic behavior for the potentials having second order Sobolev derivatives. In Section IV we specialize the results of Section III for the case of the Wiener-Fourier series representation. We prove that if the potential has first order Sobolev derivatives, then the convergence is \( o(1/n^2) \). Then, we show that if the potential has second order Sobolev derivatives, then the convergence is \( O(1/n^3) \) and we also provide the exact expression for the corresponding convergence constant. We illustrate the derived asymptotic convergence constants for the simple case of the harmonic oscillator and, in Section V, we summarize and discuss our results.

II. THE PARTIAL AVERAGING STRATEGY

A. Description of the method

In this section, we shall give a short review of the partial averaging method with the sole purpose of establishing the notation. For a more complete discussion, the reader should consult Ref. [1] and the cited bibliography. The starting point is the Feynman-Kać formula

\[
\frac{\rho(x,x';\beta)}{\rho_{fp}(x,x';\beta)} = \mathbb{E} \left\{ -\beta \int_0^1 V[x_r(u) + \sigma B_u^0] \, du \right\},
\]

where \( \rho(x,x';\beta) \) is the density matrix for a monodimensional canonical system characterized by the inverse temperature \( \beta = 1/(k_BT) \) and made up of identical particles of mass \( m_0 \) moving in the potential \( V(x) \). The stochastic element that appears in Eq. (1), \( \{B_u^0, u \geq 0\} \), is a so-called standard Brownian bridge defined as follows: if \( \{B_u, u \geq 0\} \) is a standard Brownian motion starting at zero, then the Brownian bridge is the stochastic process \( \{B_u \mid B_1 = 0, 0 \leq u \leq 1\} \) i.e., a Brownian motion conditioned on \( B_1 = 0 \). In this paper, we shall reserve the symbol \( \mathbb{E} \) to denote the expected value (average value) of a certain random variable against the underlying probability measure of the Brownian bridge \( B_u^0 \). To complete the description of Eq. (1), we set \( x_r(u) = x + (x' - x)u \) (called the reference path), \( \sigma = (\hbar^2 \beta/m_0)^{1/2} \), and let \( \rho_{fp}(x,x';\beta) \) denote the density matrix for a similar free particle.

The generalization of the Eq. (1) to a \( d \)-dimensional system is straightforward. The symbol \( B_u^0 \) now denotes a \( d \)-dimensional standard Brownian bridge, which is a vector \( \{B_{u,1}^0, B_{u,2}^0, \ldots, B_{u,d}^0\} \) with the components being independent standard Brownian bridges. The symbol \( \sigma \) stands for the vector \( \{\sigma_1, \sigma_2, \ldots, \sigma_d\} \) with components defined by \( \sigma_i^2 = \hbar^2 \beta/m_{0,i} \), while the product \( \sigma \sigma^T \) is interpreted as the \( d \)-dimensional vector of components \( \sigma_i \sigma_{j,i} \).

Finally, \( x \) and \( x' \) are points in the configuration space \( \mathbb{R}^d \) while \( x_r(u) = x + (x' - x)u \) is a line in \( \mathbb{R}^d \) connecting the points \( x \) and \( x' \). In this paper, we shall conduct the proofs for monodimensional systems and only state the easily obtainable \( d \)-dimensional results.

The most general series representation of the Brownian bridge is given by the Ito-Nisio theorem the statement of which is reproduced below. Assume given \( \{\lambda_k(\tau)\}_{k \geq 1} \) a system of functions on the interval \([0,1]\), which, together with the constant function \( \lambda_0(\tau) = 1 \), makes up an orthonormal basis in \( L^2[0,1] \). Let

\[
\Lambda_k(t) = \int_0^t \lambda_k(u) \, du.
\]

If \( \Omega \) is the space of infinite sequences \( \bar{a} \equiv (a_1, a_2, \ldots) \) and

\[
P[\bar{a}] = \prod_{k=1}^\infty \mu(a_k)
\]
is the probability measure on \( \Omega \) such that the coordinate maps \( \bar{a} \to a_k \) are independent identically distributed (i.i.d.) variables with distribution probability

\[
\mu(a_k \in A) = \frac{1}{\sqrt{2\pi}} \int_A e^{-z^2/2} \, dz,
\]

then

\[
B_u^n(\bar{a}) = \sum_{k=1}^\infty a_k \Lambda_k(u), \quad 0 \leq u \leq 1
\]
is equal in distribution to a standard Brownian bridge. Moreover, the convergence of the above series is almost surely uniform on the interval \([0, 1]\).

Using the Ito-Nisio representation of the Brownian bridge, the Feynman-Kac formula (1) takes the form

\[
\rho(x, x'; \beta) = \int_\Omega \rho_{fp}(x, x'; \beta) \exp \left\{ -\beta \int_0^1 V \left[ x_r(u) \right] \right\} \, d\mu(a_n).
\]

The independence of the coordinates \( a_k \), which physically amounts to choosing those representations in which the kinetic energy operator is diagonal, is the key to the use of the partial averaging method. Denoting by \( E_n \) the average over the coefficients beyond the rank \( n \), the partial averaging formula reads

\[
\rho_{fp}(x, x'; \beta) = \int_\mathbb{R} \lambda(a_1) \ldots \int_\mathbb{R} \lambda(a_n) \times \exp \left\{ -\beta \int_0^1 V \left[ x_r(u) + \sigma \sum_{k=1}^\infty a_k \Lambda_k(u) \right] \, du \right\}.
\]

To make more sense of the above formula, it is convenient to use the notation introduced in Ref. 3

\[
S_u^n(\bar{a}) = \sum_{k=1}^n a_k \Lambda_k(u) \quad \text{and} \quad B_u^n(\bar{a}) = \sum_{k=n+1}^\infty a_k \Lambda_k(u),
\]

which denote the \( n \)th order partial sum and \( n \)th order tail series, respectively. By construction, the random variables \( S_u^n(\bar{a}) \) and \( B_u^n(\bar{a}) \) are independent and

\[
B_u^n(\bar{a}) = \sum_{k=1}^\infty a_k \Lambda_k(u) = S_u^n(\bar{a}) + B_u^n(\bar{a}).
\]

Moreover, the variables \( B_u^n \) and \( B_r^n \) have a joint Gaussian distribution of covariances

\[
E_n(B_u^n) = \sum_{k=n+1}^\infty \Lambda_k(u)^2, \quad E_n(B_r^n) = \sum_{k=n+1}^\infty \Lambda_k(\tau)^2,
\]

and \( \gamma_n(u, \tau) = E_n(B_u^n B_r^n) = \sum_{k=n+1}^\infty \Lambda_k(u) \Lambda_k(\tau) \).

Equivalently, by using the fact that \( S_u^n(\bar{a}) \) and \( B_u^n(\bar{a}) \) are independent and their sum is \( B_u^n(\bar{a}) \), one may evaluate the above series to be

\[
E_n(B_u^n)^2 = E(B_u^n)^2 - \sum_{k=1}^n \Lambda_k(u)^2 = u(1-u) - \sum_{k=1}^n \Lambda_k(u)^2,
\]

\[
E_n(B_r^n)^2 = E(B_r^n)^2 - \sum_{k=1}^n \Lambda_k(\tau)^2 = \tau(1-\tau) - \sum_{k=1}^n \Lambda_k(\tau)^2,
\]

and

\[
\gamma_n(u, \tau) = E(B_u^n B_r^n) - \sum_{k=1}^n \Lambda_k(u) \Lambda_k(\tau) = \min(u, \tau) - u \tau - \sum_{k=1}^n \Lambda_k(u) \Lambda_k(\tau).
\]

The computation of \( E(B_u^n)^2, E(B_r^n)^2, \) and \( E(B_u^n B_r^n) \) is straightforward and is performed in Appendix A.

Going back to Eq. (6), one inverts the order of integration in the exponent and computes

\[
E_n \int_0^1 du V(x_r(u) + \sigma B_u^n(\bar{a})) = \int_\mathbb{R} \frac{1}{\sqrt{2\pi T_n^2(u)}} \exp \left\{ -\frac{z^2}{2T_n^2(u)} \right\} \, V(y + z) \, dz,
\]

with \( \Gamma_n(u) \) defined by

\[
\Gamma_n(u) = \sigma^2 E_n(B_u^n)^2 = \sigma^2 \left[ u(1-u) - \sum_{k=1}^n \Lambda_k(u)^2 \right].
\]

In deducing Eq. (6), one uses the fact that the variable \( B_u^n \) has a Gaussian distribution of variance \( E_n(B_u^n)^2 \). To summarize, we define the \( n \)th order partial averaging approximation to the diagonal density matrix by the formula

\[
\rho_{fp}(x, x'; \beta) = \int_\mathbb{R} \lambda(a_1) \ldots \int_\mathbb{R} \lambda(a_n) \times \exp \left\{ -\beta \int_0^1 V \left[ x_r(u) + \sigma \sum_{k=1}^n a_k \Lambda_k(u) \right] \, du \right\}.
\]
was found that \( \int_0^1 \Gamma^2(u)du \) attains its unique minimum

\[
\sigma^2 \left( \frac{1}{6} - \sum_{k=1}^{n} \frac{1}{\pi^2 k^2} \right)
\]
on the cosine-Fourier basis \( \{\lambda_k(\tau) = \sqrt{2} \cos(k \pi \tau); \ k \geq 1\} \). The corresponding series representation for the Brownian bridge is the Wiener-Fourier construction

\[
B^0_u(\bar{a}) \equiv \sqrt{\frac{2}{\pi^2}} \sum_{k=1}^{\infty} a_k \sin(k \pi u) / k, \ 0 \leq u \leq 1
\]

and was used by Doll and Freeman in their definition of the Fourier Path Integral method. Though their work was based on arguments other than those presented here, we consider that the name of Wiener-Fourier Path Integral (WFPI) method is more appropriate because the random series

\[
a_0 u + \sqrt{\frac{2}{\pi^2}} \sum_{k=1}^{\infty} a_k \sin(k \pi u) / k, \ 0 \leq u \leq 1
\]

was historically the first explicit construction of a standard Brownian motion and was due to Wiener.

**B. Mathematical considerations**

In this subsection, we discuss the classes of basis \( \{\lambda_k(u)\}_{k \geq 1} \) as well as the classes of smooth enough potentials for which we study the asymptotic convergence. Anticipating later results from this paper, the rate of convergence of the partial averaging sequence of approximations of the density matrix will be shown to depend solely on the properties of the function \( \gamma_n(u, \tau) \) defined by Eq. (7). Regarded as an integral kernel, the function \( \gamma_n(u, \tau) \) defines a positive definite quadratic form on \( L^2([0, 1]) \), that is

\[
\int_0^1 \int_0^1 \gamma_n(u, \tau) f(u) f(\tau) dud\tau \geq 0, \ \forall f \in L^2([0, 1]).
\]

It is but a simple exercise to verify that in general \( \gamma_n(u, \tau)^k \) defines such a positive definite quadratic form for all integers \( k \geq 1 \). In particular, we are interested in the convergence properties of \( \gamma_n(u, \tau)^2 \).

In this paper, we shall restrict our discussion to those basis \( \{\lambda_k(u)\}_{k \geq 1} \) for which there is a distribution \( g_2(u, \tau) \) such that (i)

\[
\lim_{n \to \infty} \frac{\int_0^1 \int_0^1 \gamma_n(u, \tau)^2 f(u)f(\tau) dud\tau}{\int_0^1 \int_0^1 \gamma_n(u, \tau)^2 dud\tau} = g_2(u, \tau)
\]
in the sense of distributions and (ii) \( g_2(u, \tau) \) defines an integral kernel on \( L^2([0, 1]) \) that is strictly positive definite. By convergence in the sense of distributions, we understand

\[
\lim_{n \to \infty} \frac{\int_0^1 \int_0^1 \gamma_n(u, \tau)^2 h(u, \tau) dud\tau}{\int_0^1 \int_0^1 \gamma_n(u, \tau)^2 dud\tau} = \int_0^1 \int_0^1 g_2(u, \tau) h(u, \tau) dud\tau
\]

for all continuous functions \( h(u, \tau) \), while the strictly positive definiteness of \( g_2(u, \tau) \) is the statement

\[
\int_0^1 \int_0^1 g_2(u, \tau) f(u)f(\tau) dud\tau = 0 \iff f = 0 \text{ a.s.}
\]

We mention that it is not clear if in fact these two conditions are satisfied for all basis \( \{\lambda_k(u)\}_{k \geq 1} \). However, the reader may always verify them for the problem at hand. We prove in Appendix B that for the Wiener-Fourier basis

\[
\lim_{n \to \infty} \frac{\int_0^1 \int_0^1 \gamma_n(u, \tau)^2 dud\tau}{\int_0^1 \int_0^1 \gamma_n(u, \tau)^2 dud\tau} = \delta(u - \tau)
\]
in the sense of distributions. Moreover, \( \delta(u - \tau) \) is indeed strictly positive definite because

\[
\int_0^1 \int_0^1 \delta(u - \tau) f(u)f(\tau) dud\tau = \int_0^1 f(u)^2 du
\]
is zero if and only if \( f = 0 \) a.s.

A special category of basis \( \{\lambda_k(u)\}_{k \geq 1} \) are those for which the primitives \( A_k(u) \) do not change sign. An example is furnished by the Haar wavelet basis, which generates the so called Lévy-Ciesielski representation of the Brownian bridge. For such basis, the functions \( \gamma_n(u, \tau) \) are positive and we shall further assume that there is a distribution \( g_1(u, \tau) \) such that (i)

\[
\lim_{n \to \infty} \frac{\int_0^1 \int_0^1 \gamma_n(u, \tau) dud\tau}{\int_0^1 \int_0^1 \gamma_n(u, \tau) dud\tau} = g_1(u, \tau)
\]
in the sense of distributions and (ii) \( g_1(u, \tau) \) defines an integral kernel on \( L^2([0, 1]) \) that is strictly positive definite. We analyze this category of basis separately because there are more general convergence results available for them.

In the second part of this subsection, we shall discuss the class of potentials for which the convergence is analyzed. For sure, the analysis must be restricted to those potentials for which the Feynman-Kac formula holds and for which the method does in fact converge. The Feynman-Kac formula is known to hold for a quite large class of potentials which is called the Kato class. On the other hand, it has been proven that the partial averaging method is convergent for all series representations and for all Kato-class potentials that have finite Gaussian transform. We provide below the mathematical definition of this class. The readers who find this definition meaningless might get a better insight about
the nature of the potentials in this class by studying the
examples we later provide. To arrive at the definition of
the Kato class, we let
\[
g(y) = \begin{cases} 
1, & d = 1, \\
\frac{\ln \|y\|^{1-d}}{\|y\|^{2-d}} & d = 2, \\
\frac{\ln \|y\|^{1-d}}{\|y\|^{2-d}} & d \geq 3,
\end{cases}
\]
and define the Kato class \(K_d\) as the set of all measurable functions \(f : \mathbb{R}^d \to \mathbb{R}\) such that
\[
\lim_{\alpha \to 0} \sup_{x \in \mathbb{R}^d} \int_{\|x-y\| \leq \alpha} |f(y)g(x-y)| dy = 0. \tag{15}
\]
We also say that \(f\) is in \(K^d_{\text{loc}}\) if \(1_D f \in K_d\) for all bounded domains \(D \subset \mathbb{R}^d\). We say that \(V(x)\) is a Kato-class potential if its negative part \(V^- = \max\{0, -V\}\) is in \(K_d\) while its positive part \(V^+ = \max\{0, V\}\) is in \(K^d_{\text{loc}}\).

Roughly speaking, Eq. (15) imposes a restriction on the singularities of the potentials. As far as the chemical physicist is concerned, the standard prototype as to the nature of the singularities is the general n-body potential
\[
V(\vec{r}_1, \ldots, \vec{r}_n) = \sum_{i=1}^n \frac{a_i}{\|\vec{r}_i - \vec{R}_i\|^q} + \sum_{i,j} \frac{b_{i,j}}{\|\vec{r}_i - \vec{r}_j\|^q}, \tag{16}
\]
where the individual particles are assumed to move in the usual tridimensional space. Using the observation that both \(K_d\) and \(K^d_{\text{loc}}\) classes are linear spaces and also using Proposition 4.3 of Ref. [20], the reader may prove that the potentials of the form given by Eq. (16) are in the class \(K_d\) for all \(q < 2\). Such potentials include for instance the coulombic potentials as they appear in electronic structure calculations and for which \(q = 1\). Remark that the singularities in Eq. (16) can be oriented upward or downward. It does not make any difference as to the validity of the Feynman-Kač formula as well as the convergence of the partial averaging method.

Another important example of Kato-class potentials are the functions \(V(x)\) that are continuous and bounded from below. It is trivial to verify that if \(c_1 \geq 0\) and \(c_2 \geq 0\) are some nonnegative numbers and \(V_1(x)\) and \(V_2(x)\) are Kato-class potentials, then \(c_1 V_1(x) + c_2 V_2(x)\) is also a Kato-class potential. Using this observation, one may argue that any ab initio potential obtained at the level of the Born-Oppenheimer approximation must be a Kato-class potential. This is so because it can usually be written as a sum between a \(K_d\) potential of the type given by Eq. (16) (the internuclear repulsion term) and a continuous and bounded from below potential (this term arises from the electron-nuclear and electron-electron interactions). More generally, even for strongly ionic systems, one notices that the Born-Oppenheimer potential can have at most coulombic negative singularities and therefore it is of Kato-class.

Many of the properties of the Kato-class potentials were enumerated by Aizenman and Simon. As argued by them, the Kato-class is the standard prototype as to the nature of the potentials in this class by studying the examples we later provide. To arrive at the definition of

\[
\int_D |V(x)| dx = \int_{\mathbb{R}^d} 1_D |V(x)| dx < \infty
\]
for all bounded domains \(D \subset \mathbb{R}^d\). Because of this restriction, the Leonard-Jones potential as well as some other empirical potentials are not included in the Kato-class due to the \(r^{-12}\) singularity. Even if the Feynman-Kač formula may be well defined for such potentials with positive non-integrable singularities, it is not clear if the computed answer is the Green’s function of the corresponding Bloch equation. However, as far as the chemical physicist is concerned such issues are hardly of any relevance because the Kato class comprises all potentials of physical interest. The Leonard-Jones potential can be brought into the Kato-class by truncation or other approximations.

The condition that the potentials have finite Gaussian transform can be formulated as follows. For all vectors \(\alpha = (\alpha_1, \ldots, \alpha_d) \in \mathbb{R}^d\) of strictly positive components, we consider the Gaussian measure
\[
d\mu_\alpha(z) = \left(\prod_{i=1}^d \frac{1}{\sqrt{2\pi\alpha_i}}\right)^{1/2} \exp \left(- \sum_{i=1}^d \frac{z_i^2}{2\alpha_i}\right) dz_1 \cdots dz_d. \tag{17}
\]
Then, a potential is said to have finite Gaussian transform if
\[
\|\overline{V}_\alpha(x)\| = \int_{\mathbb{R}^d} |V(x+z)| d\mu_\alpha(z) < \infty, \tag{18}
\]
for all \(x \in \mathbb{R}^d\) and \(\alpha \in \mathbb{R}^d_+\). Let us notice that from the practical point of view, this additional condition is hardly a restriction. The potentials used in actual simulations are usually a sum between the Born-Oppenheimer interatomic potential and a constraining potential. The first one always has a finite Gaussian transform. The second one is added in order to ensure that the partition function is finite
\[
Z(\beta) < \infty, \quad \forall \beta > 0
\]
and is intended to simulate, for example, the effect of the container in which a reaction takes place. For this purpose one usually uses a continuous and bounded from below potential, which is, of course, a Kato-class potential. If, for instance, the potential increases to infinity slower than any exponential \(\exp(c|x|^2)\) with \(c > 0\), then it has a finite Gaussian transform. But this is hardly a restriction since the typical constraining potentials are polynomials.

Under these conditions, it was shown that the partial averaging sequence of approximations is convergent to the correct Feynman-Kač result (which by itself is properly defined) at least as far as the convergence of the
density matrix and the partition function is concerned. However, we expect that the rate of convergence depends on the smoothness of the potential. As mentioned in the introduction, we are interested in establishing the class of potentials for which the fastest convergence is achieved. While the maximal class depends upon the specific series representation, we shall see that there is a sufficiently large class of potentials for which all series representations achieve their fastest asymptotic convergence.

Theorem 3.b) of Ref. [19] says that in order to verify that a potential has a finite Gaussian transform, it is enough to verify that

$$|V|_n(x_0) = \int_{\mathbb{R}^d} |V(x_0 + z)| \, d\mu_\alpha(z) < \infty,$$

(19)

for all $\alpha \in \mathbb{R}^d_+$ and an arbitrarily given $x_0 \in \mathbb{R}^d$. If we choose $x_0 = 0$, then the set of potentials having finite Gaussian transform is the set $\cap_\alpha L^1_\alpha(\mathbb{R}^d)$, where $L^1_\alpha(\mathbb{R}^d)$ is the space of functions $f$ for which the weighted norm

$$\|f\|_{1,\alpha} = \int_{\mathbb{R}^d} |f(z)| \, d\mu_\alpha(z)$$

(20)

is finite. By Theorem 3.a) of Ref. [19], $L^1_\alpha(\mathbb{R}^d) \subset L^1_{\infty,\alpha}(\mathbb{R}^d)$ and conversely, one may argue that a function has finite Gaussian transform if it is locally integrable and its modulus increases slower than any Gaussian at infinity.

However, in this paper we shall assume that the potential $V(x)$ lies in the set $\cap_\alpha L^2_\alpha(\mathbb{R}^d)$, where $L^2_\alpha(\mathbb{R}^d)$ is the space of functions $f$ for which the weighted norm

$$\|f\|_{2,\alpha} = \left( \int_{\mathbb{R}^d} f(z)^2 \, d\mu_\alpha(z) \right)^{1/2}$$

(21)

is finite. Since the measure $d\mu_\alpha(z)$ is a probability measure, one may apply the Cauchy–Schwarz inequality and see that $\|f\|_{1,\alpha} \leq \|f\|_{2,\alpha}$, so that $L^2_\alpha(\mathbb{R}^d) \subset L^1_\alpha(\mathbb{R}^d)$ and $\cap_\alpha L^2_\alpha(\mathbb{R}^d) \subset \cap_\alpha L^1_\alpha(\mathbb{R}^d)$. Therefore, the class of potentials discussed in the present paragraph have finite Gaussian transform. We remind the reader that $L^2_\alpha(\mathbb{R}^d) \subset L^\infty_{\infty,\alpha}(\mathbb{R}^d)$ and that the spaces $L^2_\alpha(\mathbb{R}^d)$ are Hilbert spaces.

Still, the class of potentials introduced in the previous paragraph is not smooth enough for the purpose of studying the asymptotic convergence. Later in the paper, we shall see that natural classes of smooth enough potentials are intersections of weighted Sobolev spaces $\cap_\alpha W^{m,2}_\alpha(\mathbb{R}^d)$ for $m = 1$ or $m = 2$. Since the functions $f(x) \in L^2_\alpha(\mathbb{R}^d)$ are locally integrable, they have partial distributional derivatives of any order. The weighted Sobolev space $W^{m,2}_\alpha(\mathbb{R}^d)$ is the space of all functions $f \in L^2_\alpha(\mathbb{R}^d)$ whose partial distributional derivatives up to the order $m$ are also $L^2_\alpha(\mathbb{R}^d)$ functions. In an equivalent definition, one may argue that $f \in \cap_\alpha W^{m,2}_\alpha(\mathbb{R}^d)$ if and only if

$$f(x) \exp \left( -\sum_{i=1}^d \frac{x_i^2}{2\alpha_i^2} \right) \in W^{m,2}(\mathbb{R}^d),$$

for all $\alpha \in \mathbb{R}^d_+$, where $W^{m,2}(\mathbb{R}^d)$ is the usual Sobolev space on $\mathbb{R}^d$.

There are two main categories of Kato-class potentials which we study in this paper: those that also lie in $\cap_\alpha W^{1,2}_\alpha(\mathbb{R}^d)$ and, more restrictively, those that lie in $\cap_\alpha W^{2,2}_\alpha(\mathbb{R}^d)$. For the first class of potentials, the weighted Sobolev norms

$$\int_{\mathbb{R}^d} \left\{ V(x)^2 + \sum_{i=1}^d |\partial_i V(x)|^2 \right\} \, d\mu_\alpha(x)$$

are finite, while for the second class of potentials, the norms

$$\int_{\mathbb{R}^d} \left\{ V(x)^2 + \sum_{i=1}^d |\partial_i V(x)|^2 + \sum_{i,j} |\partial_{ij} V(x)|^2 \right\} \, d\mu_\alpha(x)$$

are finite. These requirements impose further restrictions on the singularities of the Kato-class potentials. We leave it for the reader to show by explicit computation that the potentials of the form given by Eq. (16) lie in the $\cap_\alpha W^{1,2}_\alpha(\mathbb{R}^3)$ space if and only if $q < 1/2$ and in the $\cap_\alpha W^{2,2}_\alpha(\mathbb{R}^3)$ space if and only if $q < -1/2$. For another example, a general 3-body potential of the form given by the Eq. (16) but where the inter-particle potential is replaced with the Morse potential lies also in the $\cap_\alpha W^{2,2}(\mathbb{R}^3)$ space.

III. ASYMPTOTIC CONVERGENCE OF THE PARTIAL AVERAGING METHOD

In this section, we shall establish several general convergence theorems valid for all series representations and for smooth potentials. While for most of the paper we adopt a rigorous mathematical style, we shall not provide a formal proof of the key conjecture expressed by Eqs. (25) and (27). Instead, we shall try to present arguments to support this plausible assertion within reasonable doubt and then explore its implications.

We start by defining

$$U_n(x, x', \beta; \bar{a}) = \int_0^1 \nabla_{u,n} |x_r(u) + \sum_{k=1}^n a_k \Lambda_k(u)| \, du$$

and

$$U_\infty(x, x', \beta; \bar{a}) = \int_0^1 \nabla |x_r(u) + \sum_{k=1}^\infty a_k \Lambda_k(u)| \, du.$$
and in fact, 
\[
\lim_{n \to \infty} U_n(x, x', \beta; \bar{a}) = U_{\infty}(x, x', \beta; \bar{a}),
\]
(23)
as shown by Theorem 1 of Ref. [14]. To continue with the introduction of the notations, we define
\[
X_n(x, x', \beta; \bar{a}) = \rho_{fp}(x, x'; \beta) \exp[-\beta U_n(x, x', \beta; \bar{a})]
\]
and
\[
X_{\infty}(x, x', \beta; \bar{a}) = \rho_{fp}(x, x'; \beta) \exp[-\beta U_{\infty}(x, x', \beta; \bar{a})],
\]
Then, we have
\[
\rho(x, x'; \beta) = \mathbb{E}[X_{\infty}(x, x', \beta; \bar{a})]
\]
(24)
and
\[
\rho_n^{PA}(x, x'; \beta) = \mathbb{E}[X_n(x, x', \beta; \bar{a})],
\]
(25)
respectively.

A little algebra shows that
\[
\mathbb{E}_n X_n(x, x', \beta; \bar{a}) - X_n(x, x', \beta; \bar{a}) = X_n(x, x', \beta; \bar{a})
\times \mathbb{E}_n \left\{ e^{-\beta[U_{\infty}(x, x', \beta; \bar{a}) - U_n(x, x', \beta; \bar{a})]} \right\}
\]

However, for large n, we can expand the exponential in a Taylor series and retain the first non-vanishing positive term in the series, which is also the one that controls the asymptotic convergence. We have:
\[
\mathbb{E}_n X_n(x, x', \beta; \bar{a}) - X_n(x, x', \beta; \bar{a}) - X_n(x, x', \beta; \bar{a}) \approx X_n(x, x', \beta; \bar{a})
\times \frac{\beta^2}{2} \mathbb{E}_n [U_{\infty}(x, x', \beta; \bar{a}) - U_n(x, x', \beta; \bar{a})]^2.
\]
(26)

From now on, if \(A_n > 0\) and \(B_n > 0\), we interpret \(A_n \approx B_n\) to mean
\[
\lim_{n \to \infty} A_n / B_n = 1,
\]
while \(A_n \lesssim B_n\) is interpreted to mean
\[
\limsup_{n \to \infty} A_n / B_n \leq 1.
\]
The error in the equation (26) is of the order
\[
\frac{\beta^3}{3!} \mathbb{E}_n [U_{\infty}(x, x', \beta; \bar{a}) - U_n(x, x', \beta; \bar{a})]^3,
\]
which decays at a faster rate than the local variance
\[
\mathbb{E}_n [U_{\infty}(x, x', \beta; \bar{a}) - U_n(x, x', \beta; \bar{a})]^2.
\]
Therefore, the use of the symbol \(\approx\) is justified any time the local variance is not zero. However, this property is true for almost all \(\bar{a}\) whenever the potential is not constant. In Eq. (26), the term of order one in the Taylor expansion cancels because of the identity (22), so the asymptotic behavior is dictated by the local variance of the function \(U_{\infty}(x, x', \beta; \bar{a})\). The Eq. (26) is expected to be true for all potentials \(V(x) \in \cap_n L_2^2(\mathbb{R})\) which are not constant and, from now on, we shall assume that the potential satisfies these criteria. Taking the total expectation \(\mathbb{E}\) in Eq. (26) and remembering that \(X_n(x, x', \beta; \bar{a})\) does not depend upon the coefficients beyond the rank \(n\), we obtain
\[
\rho(x, x'; \beta) - \rho_n^{PA}(x, x'; \beta) \approx \frac{\beta^2}{2} \mathbb{E} \left\{ X_n(x, x', \beta; \bar{a}) \times [U_{\infty}(x, x', \beta; \bar{a}) - U_n(x, x', \beta; \bar{a})]^2 \right\}.
\]
(27)

### A. Potentials having first order Sobolev derivatives

If \(V(x) \in \cap_n W_1^2(\mathbb{R})\), Eq. (27) and Eq. (30) of Appendix C show that
\[
\mathbb{E}_n T_n'(x, x', \beta; \bar{a}) \leq \mathbb{E}_n \left\{ U_{\infty}(x, x', \beta; \bar{a}) - U_n(x, x', \beta; \bar{a}) \right\}^2 \leq \mathbb{E}_n T_n(x, x', \beta; \bar{a}),
\]
(28)
where \(T_n(x, x', \beta; \bar{a})\) and \(T_n(x, x', \beta; \bar{a})\) are positive functions defined by the equations
\[
T_n'(x, x', \beta; \bar{a}) = \sigma^2 \int_0^1 du \int_0^1 d\tau \gamma_n(u, \tau) V_{u,n}[x_r(u)]
+ \sigma S_n^2(u, \tau) V_{u,n}[x_r(u)] + \sigma S_n^2(\tau),
\]
(29)
and
\[
T_n(x, x', \beta; \bar{a}) = \sigma^2 \int_0^1 du \int_0^1 d\tau \gamma_n(u, \tau) V'[x_r(u)]
+ \sigma B_n^2(\tau) V'[x_r(\tau)] + \sigma B_n^2(\tau),
\]
(30)
respectively. Here, \(V'(x)\) denotes the first order derivative of \(V(x)\), while \(V_{u,n}(x)\) is the first order derivative of \(V_{u,n}(x)\).

With the help of the functions \(T_n'(x, x', \beta; \bar{a})\) and \(T_n(x, x', \beta; \bar{a})\) and of the equation (20) one may write
\[
\frac{\beta^2}{2} \mathbb{E}_n \left\{ X_n(x, x', \beta; \bar{a}) T_n'(x, x', \beta; \bar{a}) \right\} \lesssim \mathbb{E}_n X_n(x, x', \beta; \bar{a}) - X_n(x, x', \beta; \bar{a}) \lesssim \frac{\beta^2}{2} \mathbb{E}_n \left\{ X_n(x, x', \beta; \bar{a}) T_n(x, x', \beta; \bar{a}) \right\},
\]
(31)
where we used the fact that the function \(X_n(x, x', \beta; \bar{a})\) does not depend upon the coefficients beyond the rank \(n\) and thus, it can be placed inside the \(\mathbb{E}_n\) sign. Now, taking the total expectation \(\mathbb{E}\) in the above equation, we obtain
\[
\frac{\beta^2}{2} \mathbb{E} \left\{ X_n(x, x', \beta; \bar{a}) T_n'(x, x', \beta; \bar{a}) \right\} \lesssim \rho(x, x'; \beta) - \rho_n^{PA}(x, x'; \beta) \lesssim \frac{\beta^2}{2} \mathbb{E} \left\{ X_n(x, x', \beta; \bar{a}) T_n(x, x', \beta; \bar{a}) \right\},
\]
(32)
Moreover, due to the relation \(23\), we have
\[
\Delta X_n(x, x', \beta; \bar{a}) = X_n(x, x', \beta; \bar{a}) - X_\infty(x, x', \beta; \bar{a}) \to 0
\]
as \(n \to \infty\) and we expect that
\[
\lim_{n \to \infty} \frac{\mathbb{E}[\Delta X_n(x, x', \beta; \bar{a}) T_n(x, x', \beta; \bar{a})]}{\mathbb{E}[X_\infty(x, x', \beta; \bar{a}) T_n(x, x', \beta; \bar{a})]} = 0,
\]
because the function \(T_n(x, x', \beta; \bar{a})\) is positive while \(X_\infty(x, x', \beta; \bar{a})\) is strictly positive. Therefore, the decay of \(\Delta X_n(x, x', \beta; \bar{a})\) to zero makes the numerator converge to zero at a faster rate than the denominator. A relation similar to the one above holds for the function \(T_n'(x, x', \beta; \bar{a})\) and consequently, we may replace the estimate \([22]\) with
\[
\frac{\beta^2}{2} \mathbb{E}[X_\infty(x, x', \beta; \bar{a}) T_n'(x, x', \beta; \bar{a})] \\
\leq \rho(x, x'; \beta) - \rho_n^{PA}(x, x'; \beta) \\
\leq \frac{\beta^2}{2} \mathbb{E}[X_\infty(x, x', \beta; \bar{a}) T_n(x, x', \beta; \bar{a})].
\]

With these preparations, we are able to state the following theorem:

**Theorem 1** Assume \(V(x)\) is a Kato-class potential that lies in \(C^2(\mathbb{R})\). Then,
\[
\rho(x, x'; \beta) - \rho_n^{PA}(x, x'; \beta) \\
\leq \frac{\beta^2}{2} \int_0^1 du \int_0^1 d\tau \gamma_n(u, \tau) K^{\beta}_{x,x'}(u, \tau), \tag{34}
\]
where
\[
K^{\beta}_{x,x'}(u, \tau) = \sigma^2 \mathbb{E}\{X_\infty(x, x'; \beta; \bar{a}) V'[x_\tau(u) + \sigma B^0_n(\bar{a})] \\
\times V'[x_\tau(\tau) + \sigma B^0_n(\bar{a})]\} \tag{35}
\]

If in addition \(\gamma_n(u, \tau) \geq 0\), then the following stronger result holds
\[
\rho(x, x'; \beta) - \rho_n^{PA}(x, x'; \beta) \approx \frac{\beta^2}{2} \left[ \int_0^1 du \int_0^1 d\tau \gamma_n(u, \tau) \right] \\
\times \left[ \int_0^1 du \int_0^1 d\tau g_1(u, \tau) K^{\beta}_{x,x'}(u, \tau) \right]. \tag{36}
\]

**Proof.** The first part of the theorem follows directly from Eqs. \(29\) and \(33\), by mere substitution. In order to prove the second part of the theorem, one divides the terms in Eq. \(33\) by
\[
\int_0^1 du \int_0^1 d\tau \gamma_n(u, \tau)
\]
and then uses Eq. \(14\) as well as the expressions \(29\) and \(30\) to show that
\[
\frac{\beta^2}{2} \lim_{n \to \infty} \frac{\mathbb{E}[X_\infty(x, x', \beta; \bar{a}) T_n'(x, x', \beta; \bar{a})]}{\mathbb{E}[X_\infty(x, x', \beta; \bar{a}) T_n(x, x', \beta; \bar{a})]} = \lim_{n \to \infty} \frac{\rho(x, x'; \beta) - \rho_n^{PA}(x, x'; \beta)}{\int_0^1 du \int_0^1 d\tau \gamma_n(u, \tau)} \int_0^1 du \int_0^1 d\tau g_1(u, \tau) K^{\beta}_{x,x'}(u, \tau). \tag{37}
\]

Equation \(37\) implies the relation \(36\) provided that the common limit is not zero or infinity. We have
\[
\int_0^1 du \int_0^1 d\tau g_1(u, \tau) K^{\beta}_{x,x'}(u, \tau) \leq \sup_{u, \tau} K^{\beta}_{x,x'}(u, \tau) < \infty,
\]
where we used the fact that the integral of \(g_1(u, \tau)\) on the set \([0,1] \times [0,1]\) is 1 as well as the fact that \(K^{\beta}_{x,x'}(u, \tau)\) is continuous on the same (compact) set, thus bounded. On the other hand, using Eq. \(35\) and the fact that the
kernel $g_1(u, \tau)$ is strictly positive definite, the equality
\[
\int_0^1 du \int_0^1 d\tau g_1(u, \tau) K_{x,x'}^\beta(u, \tau) = \sigma^2 \mathbb{E} \left\{ X_\infty(x, x', \beta; \bar{a}) \right\}
\times \int_0^1 du \int_0^1 d\tau g_1(u, \tau) V'[x_r(u) + \sigma B^0_\nu(\bar{a})] \times V'[x_r(\tau) + \sigma B^0_\nu(\bar{a})] = 0
\]
implies $V'[x_r(u) + \sigma B^0_\nu(\bar{a})] = 0$ for almost all $\bar{a}$. However, this is not possible because it contradicts the fact that the potential $V(x)$ is not constant. Therefore, the limit in Eq. (\ref{eq:37}) is finite and non-zero and the proof of the theorem is concluded. \hfill \Box

Let us notice that the asymptotic rate of convergence for the partial averaging method depends upon the nature of the basis $\{\lambda_k(u)\}_{k \geq 1}$ solely through the behavior of the kernels $\gamma_n(u, \tau)$. The kernel $K_{x,x'}^\beta(u, \tau)$ is independent of the particular basis and has the important property
\[
K_{x,x'}^\beta(1 - u, 1 - \tau) = K_{x',x}^\beta(u, \tau). \quad (39)
\]
The relation (39) can be proven as follows (without loss of generality, one may assume $\tau \leq u$):
\[
K_{x,x'}^\beta(1 - u, 1 - \tau) = \sigma^2 \int \int \rho[x, y; (1 - u)] \times \rho[y, z; (u - \tau) \beta] \rho[z, x'; \tau \beta] V^{(1)}(y) V^{(1)}(z) \, dy \, dz
\]
\[
= \sigma^2 \int \int \rho[x', z; \tau \beta] \rho[z, y; (u - \tau) \beta] \rho[y, x; (1 - u) \beta] \times V^{(1)}(y) V^{(1)}(z) \, dy \, dz = K_{x',x}^\beta(\tau, u) = K_{x,x'}^\beta(u, \tau),
\]
where we used the symmetry of the various density matrices appearing in the above formula.

The relation (35) remains true for $d$-dimensional systems provided that $\sigma^2 = \hbar^2 \beta/(2 m_0, i)$ and redefine the kernel $K_{x,x'}^\beta(u, \tau)$ to be
\[
K_{x,x'}^\beta(u, \tau) = \int \int \rho[x, y; \tau \beta] \rho[y, z; (u - \tau) \beta] \times \rho[z, x'; (1 - u) \beta] \left\{ \sum_{i=1}^d \sigma_i^2 \partial_i V(y) \partial_i V(z) \right\} \, dy \, dz. \quad (40)
\]

B. Potentials having second order Sobolev derivatives

Theorem 1 provides a useful bound for the asymptotic rate of convergence, but gives the exact asymptotic convergence only if $\gamma_n(u, \tau) \geq 0$. In general, if these last functions are not positive, additional cancellations might occur if the potential is smooth enough. In this case, we need to establish lower and upper bounds that are sharper than those offered by Eq. (28).

It turns out that the natural class of potentials on which all series representations attain their fastest convergence is the class $\cap_n W^{2,2}_p(\mathbb{R})$. For potentials $V(x)$ in this class, Eqs. (C8) and (C10) of Appendix C provide the following bounds
\[
\mathbb{E}_n Y'_n(x, x', \beta; \bar{a}) \leq \mathbb{E}_n \left[ U_\infty(x, x', \beta; \bar{a}) - U_n(x, x', \beta; \bar{a}) \right]^2 \leq \mathbb{E}_n Y''_n(x, x', \beta; \bar{a}), \quad (41)
\]
where $Y'_n(x, x', \beta; \bar{a})$ and $Y''_n(x, x', \beta; \bar{a})$ are positive functions defined by the equations
\[
Y'_n(x, x', \beta; \bar{a}) = T'_n(x, x', \beta; \bar{a}) + \frac{\sigma^4}{2} \int_0^1 du \int_0^1 d\tau \gamma_n(u, \tau)^2 \times \nabla_{u\nu}[x_r(u) + \sigma S^0_\nu(\bar{a})] \nabla_r[n(x_r(\tau) + \sigma S^0_\nu(\bar{a}))] \quad (42)
\]
and
\[
Y''_n(x, x', \beta; \bar{a}) = \frac{1}{2} \left[ T''_n(x, x', \beta; \bar{a}) + T_n(x, x', \beta; \bar{a}) \right], \quad (43)
\]
respectively. Here, $\nabla'_n(x)$ denotes the second derivative of the averaged potential $V'_n(x)$. By replacing the functions $Y'_n(x, x', \beta; \bar{a})$ and $Y''_n(x, x', \beta; \bar{a})$ in Eq. (28) and taking the total expectation $\mathbb{E}$, one deduces the following sharper version of Eq. (32):
\[
\frac{\beta^2}{2} \mathbb{E} \left[ X_n(x, x', \beta; \bar{a}) \right] \leq Y'_n(x, x', \beta; \bar{a}) \leq \frac{\beta^2}{2} \mathbb{E} \left[ X_n(x, x', \beta; \bar{a}) \right] + \frac{\sigma^4}{2} \int_0^1 du \int_0^1 d\tau \gamma_n(u, \tau)^2 \times \nabla_{u\nu}[x_r(u) + \sigma S^0_\nu(\bar{a})] \nabla_r[n(x_r(\tau) + \sigma S^0_\nu(\bar{a}))]. \quad (44)
\]

In deducing Eq. (44), one should remember that the functions $X_n(x, x', \beta; \bar{a})$ do not depend upon the coefficients $a_k$ with $k \geq n + 1$ and, therefore, $\mathbb{E} \left[ X_n Y'_n \right] = \mathbb{E} \left[ X_n \mathbb{E} \left[ Y'_n \right] \right]$ and $\mathbb{E} \left[ Y'_n Y''_n \right] = \mathbb{E} \left[ X_n \mathbb{E} \left[ Y''_n \right] \right]$.

In the next few paragraphs we prove that the signs $\mathbb{E} \left[ X_n Y'_n \right]$ and $\mathbb{E} \left[ Y'_n Y''_n \right]$ in Eq. (44) can be replaced by $\approx$ and then we prove an analog of Eq. (33). As shown by Eqs. (C11) and (C12) of Appendix C,
\[
\mathbb{E}_n Y''_n(x, x', \beta; \bar{a}) - \mathbb{E}_n Y'_n(x, x', \beta; \bar{a}) \leq \frac{\sigma^4}{2} \int_0^1 du \int_0^1 d\tau \times \gamma_n(u, \tau)^2 \left\{ \mathbb{E}_n \left[ V''(x_r(u) + \sigma B^0_\nu(\bar{a})) \right] \nu''(x_r(\tau)) \right\}
\]
\[
+ \sigma B^0_\nu(\bar{a}) \} - \nabla_t[n(x_r(u) + \sigma S^0_\nu(\bar{a})] \nabla_t[n(x_r(\tau) + \sigma S^0_\nu(\bar{a}))]. \quad (45)
\]

Using this relation together with the Eq. (28), one readily proves that
\[
\lim_{n \to \infty} \left\{ \mathbb{E} \left[ X_n(x, x', \beta; \bar{a}) \right] Y'_n(x, x', \beta; \bar{a}) \right\} \left\{ \int_0^1 du \int_0^1 d\tau \gamma_n(u, \tau)^2 \right\}
\]
\[
- \mathbb{E} \left[ X_n(x, x', \beta; \bar{a}) \right] Y''_n(x, x', \beta; \bar{a}) \right\} \int_0^1 du \int_0^1 d\tau \gamma_n(u, \tau)^2 \right\} = 0.
\]
The last relation implies

\[ \mathbb{E}[X_n(x, x', \beta; \bar{a}) Y''_n(x, x', \beta; \bar{a})] \approx \mathbb{E}[X_n(x, x', \beta; \bar{a}) Y'_n(x, x', \beta; \bar{a})], \]

provided that

\[ \lim_{n \to \infty} \mathbb{E} \left[ \int_{0}^{1} du \int_{0}^{1} d\tau g_2(u, \tau) \right] > 0. \]  

(47)

In general, if \( a_n \geq b_n \geq 0 \) are some sequences of real numbers, such that

\[ \lim_{n \to \infty} (a_n - b_n) = 0 \]

and \( \liminf_{n \to \infty} b_n > 0 \), then \( a_n \approx b_n \). Indeed,

\[ 1 \leq \lim_{n \to \infty} \frac{a_n}{b_n} = 1 + \lim_{n \to \infty} \frac{a_n - b_n}{b_n} \leq 1 + \frac{\limsup_{n \to \infty} (a_n - b_n)}{\liminf_{n \to \infty} b_n} = 1. \]

Now, to prove the relation (47) and therefore Eq. (46), we learn that

\[ \mathbb{E}[X_n(x, x', \beta; \bar{a})] \approx \mathbb{E}[X_n(x, x', \beta; \bar{a})]. \]

(48)

Theorem 2 Assume \( V(x) \) is a Kato-class potential that lies in \( \cap_n W^{2,2}_{\alpha}(\mathbb{R}) \). Then,

\[ \rho(x, x'; \beta) - \rho^n_{PA}(x, x'; \beta) \approx \frac{\beta^2}{2} \mathbb{E} \left[ \int_{0}^{1} du \int_{0}^{1} d\tau \gamma_n(u, \tau) \right. \]

\[ \times K^\beta_{x,x}(u, \tau) - \frac{1}{2} \left[ \int_{0}^{1} du \int_{0}^{1} d\tau \gamma_n(u, \tau) \right]^2 \]

\[ \times \left. \int_{0}^{1} du \int_{0}^{1} d\tau g_2(u, \tau) Q^\beta_{x,x}(u, \tau) \right\} \}

\[ \text{where } Q^\beta_{x,x}(u, \tau) = \sigma^4 \mathbb{E} \left[ X_{\infty}(x, x', \beta; \bar{a}) Y''_n(x, x', \beta; \bar{a}) \right] \times V''[x_r(u) + \sigma B^\beta_n(\bar{a})]. \]

(49)

Proof Let us notice that if \( a_n \approx b_n \), then \( a_n \approx 2b_n - a_n \). Indeed,

\[ \lim_{n \to \infty} \frac{2b_n - a_n}{a_n} = 2 \lim_{n \to \infty} \frac{b_n}{a_n} - 1 = 1. \]

Using this observation together with the equation (48), we deduce that

\[ \rho(x, x'; \beta) - \rho^n_{PA}(x, x'; \beta) \]

\[ \approx \frac{\beta^2}{2} \mathbb{E} \left[ X_{\infty}(x, x', \beta; \bar{a}) Y''_n(x, x', \beta; \bar{a}) \right], \]

(50)

where

\[ Y_n(x, x', \beta; \bar{a}) = 2Y''_n(x, x', \beta; \bar{a}) - Y'_n(x, x', \beta; \bar{a}). \]

From Eq. (42) and Eq. (43), we learn that

\[ Y_n(x, x', \beta; \bar{a}) = T_n(x, x', \beta; \bar{a}) - Z_n(x, x', \beta; \bar{a}), \]

where

\[ Z_n(x, x', \beta; \bar{a}) = \frac{\beta^2}{2} \mathbb{E} \left[ X_{\infty}(x, x', \beta; \bar{a}) Y''_n(x, x', \beta; \bar{a}) \right]. \]

If we also introduce the random variable

\[ Z'_n(x, x', \beta; \bar{a}) = \frac{\beta^2}{2} \mathbb{E} \left[ T_n(x, x', \beta; \bar{a}) - Z'_n(x, x', \beta; \bar{a}) \right]. \]

we notice that the right-hand side of Eq. (49) is precisely

\[ \frac{\beta^2}{2} \mathbb{E} \left[ X_{\infty}(x, x', \beta; \bar{a}) [T_n(x, x', \beta; \bar{a}) - Z'_n(x, x', \beta; \bar{a})] \right]. \]

Now, if the potential is linear but not constant, the theorem follows trivially because the functions \( Z_n(x, x', \beta; \bar{a}) \)
and $Z'_{n}(x, x', \beta; \bar{a})$ are identically zero. Therefore, for the remainder of the proof, we assume that the potential is not linear. Let us set

$$
\Delta Z_{n}(x, x'; \beta; \bar{a}) = Z_{n}(x, x'; \beta; \bar{a}) - Z'_{n}(x, x'; \beta; \bar{a})
$$

and notice again that the theorem follows trivially from Eq. (51) provided that

$$
\lim_{n \to \infty} \frac{E \left[ X_{\infty}(x, x', \beta; \bar{a}) \Delta Z_{n}(x, x', \beta; \bar{a}) \right]}{E \left[ X_{\infty}(x, x', \beta; \bar{a})Y_{n}(x, x', \beta; \bar{a}) \right]} = 0. \tag{52}
$$

In order to prove that the limit in the last equation is indeed zero, we observe that since $E \left[ X_{\infty}Y_{n} \right] \approx E \left[ X_{\infty}Y_{n}' \right]$ and since $Y_{n}' \geq Z_{n}$, we have

$$
\lim_{n \to \infty} \frac{E \left[ X_{\infty}(x, x', \beta; \bar{a}) \Delta Z_{n}(x, x', \beta; \bar{a}) \right]}{E \left[ X_{\infty}(x, x', \beta; \bar{a})Z_{n}(x, x', \beta; \bar{a}) \right]} \geq 1.
$$

Therefore, the limit in Eq. (52) is smaller or equal than

$$
\lim_{n \to \infty} \frac{E \left[ X_{\infty}(x, x', \beta; \bar{a}) \Delta Z_{n}(x, x', \beta; \bar{a}) \right]}{E \left[ X_{\infty}(x, x', \beta; \bar{a})Z_{n}(x, x', \beta; \bar{a}) \right]}. \tag{53}
$$

However, the limit in Eq. (53) is zero because $E \left[ X_{\infty}Z_{n} \right] \approx E \left[ X_{\infty}Z_{n}' \right]$. This last statement follows from the equality

$$
\lim_{n \to \infty} \frac{E \left[ X_{\infty}(x, x', \beta; \bar{a})Z_{n}(x, x', \beta; \bar{a}) \right]}{E \left[ X_{\infty}(x, x', \beta; \bar{a}) \right]} = \lim_{n \to \infty} \frac{E \left[ X_{\infty}(x, x', \beta; \bar{a})Z_{n}(x, x', \beta; \bar{a}) \right]}{E \left[ X_{\infty}(x, x', \beta; \bar{a}) \right]}
$$

because the above common limit is finite and non-zero by an argument similar to the one employed in the proof of Theorem 1. The proof of Theorem 2 is therefore concluded. \( \square \)

The kernel $Q_{x,x'}^{\beta}(u, \tau)$ shares most of the properties proved for $K_{x,x'}(u, \tau)$. In particular, $Q_{x,x'}^{\beta}(u, \tau)$ is symmetric at the permutation of the variables $u$ and $\tau$ and, if $\tau \leq u$,

$$
Q_{x,x'}^{\beta}(u, \tau) = \sigma^4 \int_{\mathbb{R}} \int_{\mathbb{R}} \rho(x, y; \beta \tau) \rho(y, z; (u - \tau) \beta) \times \rho(z, x'; (1 - u) \beta) V''(y) V''(z) \, dy \, dz. \tag{54}
$$

In addition, $Q_{x,x'}^{\beta}(u, \tau)$ is continuous in the variables $\tau$ and $u$ and

$$
Q_{x,x'}^{\beta}(1 - u, 1 - \tau) = Q_{x',x}^{\beta}(u, \tau). \tag{55}
$$

The equation (49) remains true for multidimensional systems provided that we define the kernel $K_{x,x'}^{\beta}(u, \tau)$ as in Eq. (49), while for the kernel $Q_{x,x'}^{\beta}(u, \tau)$ we employ the formula

$$
Q_{x,x'}^{\beta}(u, \tau) = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \rho(x, y; \beta \tau) \rho(y, z; (u - \tau) \beta) \times \rho(z, x'; (1 - u) \beta) \sum_{i,j} \sigma_i^2 \sigma_j^2 \left[ \partial_i^2 \partial_j^2 V(y) \right. \left. \times \partial_i^2 \partial_j^2 V(z) \right]. \tag{56}
$$

IV. CONVERGENCE OF THE PA-WFPI METHOD

As argued in Ref. [3], among all possible series representations, the Wiener-Fourier one is special in the sense that it has the fastest asymptotic rate of convergence. For this reason, it is of interest to establish what the asymptotic rates of convergence are for different classes of potentials. In this section, we shall show that for potentials lying in $\cap_n W^2_{\alpha,2}(\mathbb{R})$, the asymptotic rate of convergence is always better than $O(1/n^2)$, while for potentials lying in $\cap_n W^2_{\alpha,2}(\mathbb{R})$, the asymptotic rate of convergence is $O(1/n^3)$. For the latter case, we also establish the exact convergence constant.

A. Potentials with first order Sobolev derivatives

We begin the convergence analysis with the Kato-class potentials that lie in $\cap_n W^{1,2}_{\alpha,2}(\mathbb{R})$. For the Wiener-Fourier basis, we have

$$
\gamma_n(u, \tau) = \frac{2}{\pi^2} \sum_{k=n+1}^{\infty} \sin(k\pi u) \sin(k\pi \tau). \tag{57}
$$

If $f(t)$ is a square integrable function on the interval $[0, 1]$, then we have the estimate

$$
\int_0^1 \int_0^1 \gamma_n(u, \tau) f(u) f(t) \, du \, d\tau = \frac{1}{\pi^2} \sum_{k=n+1}^{\infty} \frac{1}{k^2} \left[ \sqrt{\frac{1}{\pi^2}} \int_0^1 f(u) \sin(k\pi u) \, du \right]^2 \tag{58}
$$

$$
\leq \frac{1}{\pi^2(n+1)^2} \sum_{k=n+1}^{\infty} \left[ \sqrt{\frac{1}{\pi^2}} \int_0^1 f(u) \sin(k\pi u) \, du \right]^2.
$$

Now, the first part of Theorem 1 allows us to write

$$
\rho(x, x'; \beta) - \rho^{PA}_{x,x'}(x, x'; \beta) \leq \frac{\beta^2 \sigma^2}{2} \left[ X_{\infty}(x, x', \beta; \bar{a}) \times \int_0^1 \int_0^1 \int_0^1 d\tau \gamma_n(u, \tau) V'[x_\tau(u) + \sigma B^0_{\tau}(\bar{a})] \right] \tag{59}
$$

and using Eq. (57), we obtain

$$
\lim_{n \to \infty} \frac{\beta^2 \sigma^2}{2} \left[ X_{\infty}(x, x', \beta; \bar{a}) \times \int_0^1 \int_0^1 \int_0^1 d\tau \gamma_n(u, \tau) V'[x_\tau(u) + \sigma B^0_{\tau}(\bar{a})] \right] \tag{60}
$$

$$
\lim_{n \to \infty} \frac{\beta^2 \sigma^2}{2} \left[ X_{\infty}(x, x', \beta; \bar{a}) \times \int_0^1 \int_0^1 \int_0^1 d\tau \gamma_n(u, \tau) V'[x_\tau(u) + \sigma B^0_{\tau}(\bar{a})] \right] = \sum_{k=n+1}^{\infty} \frac{1}{k^2} \left[ \sqrt{\frac{1}{\pi^2}} \int_0^1 f(u) \sin(k\pi u) \, du \right]^2.
$$

and

$$
Z_n(x, x', \beta; \bar{a}) \leq \frac{\beta^2 \sigma^2}{2\pi^2} \left[ X_{\infty}(x, x', \beta; \bar{a}) \times \int_0^1 \int_0^1 \int_0^1 d\tau \gamma_n(u, \tau) V'[x_\tau(u) + \sigma B^0_{\tau}(\bar{a})] \right] \tag{61}
$$

$$
\lim_{n \to \infty} \frac{\beta^2 \sigma^2}{2\pi^2} \left[ X_{\infty}(x, x', \beta; \bar{a}) \times \int_0^1 \int_0^1 \int_0^1 d\tau \gamma_n(u, \tau) V'[x_\tau(u) + \sigma B^0_{\tau}(\bar{a})] \right] = \sum_{k=n+1}^{\infty} \frac{1}{k^2} \left[ \sqrt{\frac{1}{\pi^2}} \int_0^1 f(u) \sin(k\pi u) \, du \right]^2.
$$
We notice that the sequence of functions \( Z_0(x, x', \beta; \bar{a}) \) is monotonically decreasing and convergent to zero. Moreover, since the functions \( \{ \sqrt{2} \sin(k \pi u) \}_{k \geq 1} \) form an orthonormal system, the Bessel inequality implies that
\[
Z_0(x, x', \beta; \bar{a}) \leq \int_0^1 V'[x_r(u) + \sigma B_0^0(\bar{a})]^2 du.
\]
We then have the inequality
\[
\mathbb{E}[X_\infty(x, x', \beta; \bar{a})Z_0(x, x', \beta; \bar{a})] \\
\leq \int_0^1 du \int \mathbb{P}(x, y; u) \rho(x, y; \beta V'(y)^2) < \infty.
\]
The last integral is finite because \( V(x) \in \cap_0 W^{1,2}(\mathbb{R}) \).
In these conditions, the dominated convergence theorem shows that
\[
\lim_{n \to \infty} \mathbb{E}[X_\infty(x, x', \beta; \bar{a})Z_n(x, x', \beta; \bar{a})] = 0,
\]
and we have just proved the following theorem

**Theorem 3** If \( V(x) \) is a Kato-class potential that lies in \( \cap_0 W^{1,2}(\mathbb{R}) \) and the basis \( \{ \lambda_k(u) \}_{k \geq 1} \) is the Wiener-Fourier basis, then
\[
\lim_{n \to \infty} (n + 1)^2 [\rho(x, x'; \beta) - \rho_n^{PA}(x, x'; \beta)] = 0. \tag{61}
\]

**Observation** The previous theorem says that the convergence is always better than \( O(1/n^2) \) [i.e., it is \( O(1/n^2) \)], but it does not say how much better. If we are interested in computing an absolute asymptotic bound, then the bound given by the relation
\[
\rho(x, x'; \beta) - \rho_n^{PA}(x, x'; \beta) \leq \frac{\beta^2 \sigma^2}{2 \pi^2 (n + 1)^2}
\]

\[
\times \mathbb{E}[X_\infty(x, x', \beta; \bar{a})Z_0(x, x', \beta; \bar{a})] \leq \frac{h^2 \beta^3}{2 \pi^2 m_0 (n + 1)^2} \tag{62}
\]

\[
\times \int_0^1 d\theta \int \mathbb{P}(x, y; \theta \beta V'(y)^2) \rho(x, y; \beta V'(y)^2) < \infty
\]
is the only choice if no additional information about the potential \( V(x) \) is available. Theorem 3 remains true as stated for multidimensional systems, while in an even more compact notation, the estimate given by Eq. 62 becomes
\[
\rho(x, x', \beta) - \rho_n^{PA}(x, x', \beta) \leq \frac{h^2 \beta^3}{2 \pi^2 (n + 1)^2}
\]

\[
\times \int_0^1 \left( x e^{-\theta \beta H} \sum_{i=1}^d \left( \frac{\partial_i V)^2}{m_{0,i}} \right) e^{-(1-\theta) \beta H} x' \right) d\theta. \tag{63}
\]

**B. Potentials having second order Sobolev derivatives**

As we have shown in Section III.B, all series representations attain their fastest asymptotic convergence on the class of potentials \( \cap_0 W^{2,2}(\mathbb{R}) \). Of course, this is also true of the Wiener-Fourier series. Moreover, since this series is optimal as asymptotic convergence, the rates of convergence established in this section set a limit on the asymptotic behavior of the partial averaging method. In this section, we prove that the asymptotic convergence of the PA-WFPI sequence of approximations to the density matrix is \( O(1/n^3) \) and we establish the corresponding convergence constant.

We start our proof by analyzing the first term in Eq. 64. Let us notice that \( \gamma_n(1 - u, 1 - \tau) = \gamma_n(u, \tau) \) because \( \sin[k \pi (1 - t)] = (-1)^k \sin(k \pi t) \). By using this relation together with Eq. 64, one computes
\[
\int_0^1 du \int_0^1 \mathbb{P}(u, \tau) K_{x,x}(u, \tau)
\]

\[
= \int_0^1 du \int_0^{1-u} \mathbb{P}(u, 1 - \tau) K_{x,x}(u, 1 - \tau)
\]

\[
= \int_0^1 du \int_0^u \mathbb{P}(u, 1 - \tau) K_{x,x}(1 - u, 1 - \tau)
\]

A little thought shows that the first term in Eq. 64 takes the form
\[
\frac{\beta^2 \pi^2}{2} \sum_{k=n+1}^\infty \int_0^1 du \int_0^1 \mathbb{P}(u, \tau) \frac{\sin(k \pi u) \sin(k \pi \tau)}{k^2} K(u, \tau), \tag{64}
\]

where
\[
K(u, \tau) = K_{x,x}(u, \tau) + K_{x,x}(\tau, u).
\]

The asymptotic rate of convergence of this first term is dictated by the decay of the terms of the series appearing in Eq. 64. By integration by parts, we shall later show that these terms are of the form \( A_k/k^4 + B_k/k^4 \), where \( \{ B_k \}_{k \geq 1} \) is a sequence convergent to zero. Because of this property, the terms \( B_k/k^4 \) do not contribute to the final asymptotic convergence, at least as far as the \( O(1/n^3) \) is concerned. Indeed, we have
\[
\lim_{n \to \infty} n^3 \sum_{k=n+1}^\infty |B_k/k^4| \leq \lim_{n \to \infty} n^3 \sum_{k=n+1}^\infty |B_k|/k^4
\]

\[
\leq \lim_{n \to \infty} \left( \sup_{k \geq n} |B_k| \right) \sum_{k \geq n} n^3/k^4
\]

\[
\leq \frac{1}{3} \lim_{n \to \infty} \left( \sup_{k \geq n} |B_k| \right) = 0,
\]

which proves our assertion. In the above, we used the inequality
\[
\sum_{k=n+1}^\infty n^3/k^4 \leq n^3 \int_n^\infty x^{-4} dx = \frac{1}{3}
\]
as well as the fact that $B_k \to 0$ implies
\[
\limsup_{n \to \infty} |B_k| = \lim_{n \to \infty} \left( \sup_{k \geq n} |B_k| \right) = 0.
\]

Now, to readily identify which of the various expressions make up the terms $B_k$ that decay to zero, the reader may employ the Riemann-Lebesgue lemma, which in our case states that if $f(t)$ is integrable, then
\[
\lim_{k \to \infty} \int_0^1 \cos(k\pi t) f(t) dt = \lim_{k \to \infty} \int_0^1 \sin(k\pi t) f(t) dt = 0.
\]

We start with the equation (65) and by integration by parts against the variable $\tau$, we obtain
\[
\frac{1}{k^2} \int_0^1 du \sin(k\pi u) \int_0^u \sin(k\pi \tau) K(u, \tau) d\tau = \\
\int_0^1 \sin(k\pi u) K(u, 0) - \cos(k\pi u) K(u, u) du
\]
\[
+ \frac{1}{k^3 \pi} \int_0^1 du \sin(k\pi u) \int_0^u \cos(k\pi \tau) \frac{\partial}{\partial \tau} K(u, \tau) d\tau.
\]

Let us focus on the first term of the relation (65). By integration by parts against $u$ we have
\[
\frac{1}{k^3 \pi} \int_0^1 \sin(k\pi u) K(u, 0) du = \frac{K(0, 0) - (-1)^k K(1, 0)}{k^2 \pi^2}
\]
\[
+ \frac{1}{k^3 \pi} \int_0^1 \cos(k\pi u) \frac{\partial}{\partial u} K(u, 0) du \tag{66}
\]

and
\[
\frac{1}{k^3 \pi} \int_0^1 \sin(k\pi u) \cos(k\pi u) K(u, u) du = \frac{1}{2k^3 \pi}
\]
\[
\times \int_0^1 \sin(2k\pi u) K(u, u) du = \frac{K(0, 0) - K(1, 1)}{4k^4 \pi^2}
\]
\[
+ \frac{1}{4k^3 \pi^2} \int_0^1 \cos(2k\pi u) \frac{\partial}{\partial u} K(u, u) du,
\]

respectively. As argued before by means of the Riemann-Lebesgue lemma, the last terms in the relations (66) and (67) do not contribute to the asymptotic rates of convergence and therefore, they will be dropped. Moreover, even the term $K(1,0)(-1)^k/k^4 \pi^2$ does not contribute to the asymptotic rate of convergence because
\[
\sum_{k=n+1}^{\infty} \frac{(-1)^k}{k^4} = \sum_{k=0}^{\infty} \frac{1}{(n+2k+1)^4} - \frac{1}{(n+2k+2)^4}
\]
\[
= \sum_{k=0}^{\infty} \int_{n+2k+1}^{n+2k+2} 4x^{-5} dx \leq 4 \int_{n+1}^{\infty} x^{-5} dx = \frac{1}{(n+1)^4}
\]
decays faster than $1/n^3$. Finally, the first term in Eq. (67) is zero because
\[
K(0, 0) = K(1, 1) = \sigma^2 \rho(x, x'; \beta) \left[V'(x)^2 + V'(x')^2\right].
\]

Now, we go back to the formula (63) and integrate by parts the last term against the variable $u$. One obtains
\[
\frac{1}{k^3 \pi} \int_0^1 du \sin(k\pi u) \int_0^u \cos(k\pi \tau) \frac{\partial}{\partial \tau} K(u, \tau) d\tau
\]
\[
= \frac{(-1)^k}{k^4 \pi^2} \int_0^1 \cos(k\pi \tau) \frac{\partial}{\partial \tau} K(1, \tau) d\tau + \frac{1}{k^4 \pi^2}
\]
\[
\times \int_0^1 \cos(k\pi u)^2 \frac{\partial^2}{\partial \tau^2} K(u, \tau) d\tau + \frac{1}{k^4 \pi^2} \tag{69}
\]
\[
\times \int_0^1 du \cos(k\pi u) \int_0^u \cos(k\pi \tau) \frac{\partial^2}{\partial \tau \partial \tau} K(u, \tau) d\tau.
\]

Again, the first and the last terms from the above expansion do not contribute to the asymptotic rate of convergence by the Riemann-Lebesgue lemma. For the last term, notice that by symmetry
\[
\int_0^1 du \cos(k\pi u) \int_0^u \cos(k\pi \tau) \frac{\partial^2}{\partial \tau \partial \tau} K(u, \tau) d\tau
\]
\[
= \frac{1}{2} \int_0^1 \int_0^1 \cos(k\pi u) \cos(k\pi \tau) \frac{\partial^2}{\partial \tau \partial \tau} K(u, \tau) d\tau du\tag{70}
\]
and then the bidimensional version of the Riemann-Lebesgue lemma applies. Therefore, the contribution of Eq. (69) to the asymptotic rate of convergence is due solely to the term
\[
\frac{1}{k^3 \pi} \int_0^1 \cos(k\pi u)^2 \frac{\partial}{\partial \tau} K(u, \tau) \bigg|_{\tau=u} du
\]
\[
= \frac{1}{2k^4 \pi^2} \int_0^1 \frac{\partial}{\partial \tau} K(u, \tau) \bigg|_{\tau=u} du + \frac{1}{2k^4 \pi^2}
\]
\[
\times \int_0^1 \cos(2k\pi u) \frac{\partial}{\partial \tau} K(u, \tau) \bigg|_{\tau=u} du
\]

Yet again, the last term of Eq. (70) does not contribute to the asymptotic rate by the same Riemann-Lebesgue lemma.

Combining everything by means of Eq. (63), we end up with the following asymptotic expression for the relation (63):
\[
\frac{\beta^2}{3\pi^3 n^3} \left[ K(0, 0) + \frac{1}{2} \int_0^1 \frac{\partial}{\partial \tau} K(u, \tau) \bigg|_{\tau=u} du \right], \tag{71}
\]
where we also used the equality
\[
\lim_{n \to \infty} \left( n^3 \sum_{k=n+1}^{\infty} \frac{1}{k^4} \right) = \frac{1}{3}.
\]

This last equality can be deduced by letting $n \to \infty$ in Eq. (135) of Appendix B.

The exact expression for the term $K(0,0)$ is given by Eq. (68). To evaluate this term
\[
\int_0^1 \frac{\partial}{\partial \tau} K(u, \tau) \bigg|_{\tau=u} du,
\]
we need to remember that the density matrix satisfies the Bloch equation
\[ -\frac{\hbar^2}{2m_0} \frac{\partial^2}{\partial x^2} \rho(x,x';\beta) + V(x') \rho(x,x';\beta) = -\frac{\partial}{\partial \beta} \rho(x,x';\beta). \]

Using the Bloch equation, one can justify by explicit calculation the following equality:
\[ \frac{\partial}{\partial \tau} K_{x,x'}^\beta(u,\tau) = \frac{\hbar^2 \sigma^2 \beta}{2m_0} \int_\mathbb{R} \int_\mathbb{R} \left\{ \frac{\partial^2}{\partial y^2} \rho(x,y;\tau \beta) \times \rho[y,z;(u-\tau)\beta] + \rho(x,y;\tau \beta) V''(y) \rho[y,z; (u-\tau)\beta] \right\} \times \rho[z,x';(1-u)\beta] V'(y) V'(z) \, dy \, dz. \]

and by repeated integration by parts against \( y \),
\[ \frac{\partial}{\partial \tau} K_{x,x'}^\beta(u,\tau) = -\frac{\hbar^2 \sigma^2 \beta}{2m_0} \int_\mathbb{R} \int_\mathbb{R} \left\{ 2 \frac{\partial}{\partial y} \rho(x,y;u \beta) V''(y) + \rho(x,y;u \beta) V''(y) \right\} \rho[y,x';(1-u)\beta] V'(y) \, dy. \]

By integration by parts of the term containing the third derivative \( V'''(x) \), we obtain
\[ \frac{\partial}{\partial \tau} K_{x,x'}^\beta(u,\tau) \bigg|_{\tau=u} = \frac{\hbar^2 \sigma^2 \beta}{2m_0} \int_\mathbb{R} \int_\mathbb{R} \left\{ \frac{\partial}{\partial y} \rho(x,y;u \beta) V'''(y) \times V''(y) dy \right\} \rho[y,x';(1-u)\beta] V'(y) \, dy. \]

A similar estimate holds for
\[ \frac{\partial}{\partial \tau} K_{x,x'}^\beta(u,\tau) \bigg|_{\tau=u}, \]
and can by obtained simply by permuting \( x \) and \( x' \). The equality
\[ \int_0^1 \int_\mathbb{R} V'(y) V''(y) \left[ \frac{\partial}{\partial y} \rho(x,y;u \beta) \right] \times \rho[y,x';(1-u)\beta] \, du = \int_0^1 \int_\mathbb{R} V'(y) V''(y) \times \rho(x',y;u \beta) \frac{\partial}{\partial y} \rho[y,x;(1-u)\beta] \, du \]

as well as the one obtained by permuting \( x \) and \( x' \) are readily obtained by use of the substitution \( u' = 1 - u \) and by use of the symmetry of the density matrices. We leave it for the reader to utilize these equalities and verify that
\[ \int_0^1 \frac{\partial}{\partial \tau} K(u,\tau) \bigg|_{\tau=u} \, du = \int_0^1 \frac{\partial}{\partial \tau} K_{x,x'}^\beta(u,\tau) \bigg|_{\tau=u} \, du + \int_0^1 \frac{\partial}{\partial \tau} K_{x',x}^\beta(u,\tau) \bigg|_{\tau=u} \, du \]
\[ \times \int_0^1 \int_\mathbb{R} \rho(x,y;u \beta) \rho[y,x';(1-u)\beta] V''(y) \, dy \, du. \]

Replacing Eq. (72) in Eq. (71), one ends up with the following expression for the first term of the equation (49):
\[ \frac{\hbar^2 \beta^3}{3 \pi^4 m_0 n^3} \left\{ \rho(x,x';\beta) \left[ V'(x)^2 + V'(x')^2 \right] + \frac{h^2 \beta}{2m_0} \times \int_0^1 \int_\mathbb{R} \int_\mathbb{R} \left\{ \frac{\partial}{\partial y} \rho(x,y;u \beta) \right\} \rho[y,x';(1-u)\beta] V'(y) V'(z) \, dy \, dz. \]

The second term in Eq. (49) is a little easier to analyze. Eq. (133) from Appendix B shows that for the Wiener-Fourier series,
\[ \lim_{n \to \infty} \frac{n^3}{\beta^2} g_n(u,\tau) = \frac{1}{3 \pi^4} \beta \delta(u-\tau) \]
in the sense of distributions. Using this equality and the relation (50), we learn that the decay of the last term of equation (49) is
\[ \frac{\beta^2}{12 \pi^4} \int_0^1 \int_\mathbb{R} \left\{ \frac{\partial}{\partial y} \rho(x,y;u \beta) \right\} \rho[y,x';(1-u)\beta] V'(y) V'(z) \, dy \, dz \]
\[ \times \int_0^1 \int_\mathbb{R} \left\{ \frac{\partial}{\partial y} \rho(x,y;u \beta) \right\} \rho[y,x';(1-u)\beta] V'(y) V'(z) \, dy \, dz. \]

Replacing Eq. (72) and Eq. (71) in Eq. (49), one ends up with the following theorem

**Theorem 4**
\[ \lim_{n \to \infty} \frac{n^3}{\beta^2} \left[ \rho(x,x';\beta) - \rho_{nA}^0(x,x';\beta) \right] \]
\[ = \frac{h^2 \beta^3}{3 \pi^4 m_0} \rho(x,x';\beta) \left[ V'(x)^2 + V'(x')^2 \right] \]
\[ + \frac{h^4 \beta^4}{12 \pi^4 m_0} \int_0^1 \int_\mathbb{R} \left\{ \frac{\partial}{\partial y} \rho(x,y;u \beta) \right\} \rho[y,x';(1-u)\beta] V'(y) V'(z) \, dy \, dz. \]

The \( d \)-dimensional analog can be deduced in a similar way by starting with Eqs. (10) and (56) and by using the \( d \)-dimensional Bloch equation. It has the expression
\[
\lim_{n \to \infty} n^3 [\rho(x, x'; \beta) - \rho^{PA}_{n}(x, x'; \beta)] = \frac{\hbar^2 \beta^3}{27} \rho(x, x'; \beta) \left\{ \sum_{i=1}^{d} \frac{[\partial_i V(x)]^2 + [\partial_i V(x')]^2}{m_{0,i}} \right\} + \frac{\hbar^4 \beta^4}{12 \pi^4} \int_{0}^{1} x e^{-\beta \theta H} \sum_{i,j=1}^{d} \frac{(\partial^2_{i,j} V)^2}{m_{0,i} m_{0,j}} e^{-\beta(1-\theta) H} x' d\theta. \tag{76}
\]

We conclude this section by numerically verifying the findings of Theorem 4 for the simple case of an harmonic oscillator. In fact, we shall verify the following corollary, which, by trace invariance, is a direct consequence of Theorem 4.

**Corollary 1**

\[
\lim_{n \to \infty} n^3 \frac{Z(\beta) - Z^{PA}_n(\beta)}{Z(\beta)} = \frac{\int_{\mathbb{R}} \rho(x; \beta) \Delta Z(x; \beta) dx}{\int_{\mathbb{R}} \rho(x; \beta) dx},
\]

where

\[
\Delta Z(x; \beta) = \frac{2 \hbar^2 \beta^3}{3 \pi^4 m_0} V'(x)^2 + \frac{\hbar^4 \beta^4}{12 \pi^4 m_0^2} V''(x)^2.
\]

The Corollary 1 gives an estimate for the relative error of the partition function as an average of a suitable estimating function. In practice, such an average can be evaluated by Monte Carlo integration if so desired.

In the remainder of this section, we shall verify the Corollary 1 for the simple case of the harmonic oscillator \(V(x) = m_0 \omega^2 x^2 / 2\). The computations are performed in atomic units for a particle of mass \(m_0 = 1\) and for the frequency \(\omega = 1\). The inverse temperature is set to \(\beta = 10\).

Since the density matrix for an harmonic oscillator is analytically known, the convergence constant for the relative error of the partition function can be evaluated directly from Corollary 1 to be

\[
c_{PA} = \frac{\int_{\mathbb{R}} \rho(x; \beta) \Delta Z(x; \beta) dx}{\int_{\mathbb{R}} \rho(x; \beta) dx} = 11.98.
\]

We can also evaluate it by studying the limit of the sequence

\[
c^{PA}_n = n^3 \frac{Z(\beta) - Z^{PA}_n(\beta)}{Z(\beta)}.
\]

In this respect, we mention that the terms \(Z^{PA}_n(\beta)\) were previously evaluated in Appendix B of Ref. 2. Also, because the even and the odd sequences \(c^{PA}_{2n}\) and \(c^{PA}_{2n+1}\) have a slightly different asymptotic behavior that generates an oscillatory pattern in plots, we choose to plot them separately.

In these conditions, the Corollary 1 says that

\[
c_{PA} = \lim_{n \to \infty} c^{PA}_n
\]

and the prediction is well verified for the harmonic oscillator, as Fig. 1 shows. We regard this numerical example as strong evidence that the analysis performed in the present paper is correct. Indeed, it is hard to believe that the exact agreement between theory and numerical analysis for the harmonic oscillator is accidental.

**V. SUMMARY AND DISCUSSION**

In this paper, we have performed a complete analysis of the asymptotic rates of convergence of the partial averaging sequence of approximations for the density matrix. We have found that there are two natural classes of potentials on which different series may achieve their fastest convergence. If the two-point correlation function \(\gamma_n(u, \tau)\) for the tail series is positive, then the natural class is \(\cap_{\alpha} W_{\alpha}^{1,2}(\mathbb{R})\) as shown by Theorem 1. More generally, all series representations achieve their fastest convergence on the space of potentials \(\cap_{\alpha} W_{\alpha}^{1,2}(\mathbb{R})\). This is the statement of Theorem 2. Moreover, in both cases, the cited theorems provide the exact asymptotic rates of convergence for arbitrary series.

In Section IV, we analyzed the special case of the Wiener-Fourier series representation. Theorem 3 asserts that the asymptotic convergence for this series is \(o(1/n^2)\) on the Kato-class potentials that lie in \(\cap_{\alpha} W_{\alpha}^{1,2}(\mathbb{R})\).
Moreover, the equations (12) and (13) provide useful (though conservative) bounds that control the absolute asymptotic error. The Wiener-Fourier series achieves its fastest asymptotic convergence on the Kato-class potentials that lie in $\cap_n W^{2,2}_n(\mathbb{R})$. This convergence is $O(1/n^3)$, with a convergence constant given by Eq. (75) for monodimensional systems and by Eq. (76) for multidimensional systems, respectively.

The present results provide a relatively complete characterization of the asymptotic convergence characteristics of the partial averaging methods. Beyond establishing sharp estimates of the convergence constants for applications where the potential energy has second-order derivatives, it should be possible to utilize the present methods to characterize the asymptotic behavior of other properties. In particular, we would speculate that it should be possible to obtain convergence constants for both the H-method and T-method energy estimators using arguments similar to those developed in the present paper. Moreover, we expect that the theorems proved in this paper will play a crucial role in establishing the asymptotic rates of convergence for the reweighted arguments similar to those developed in the present paper.

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**APPENDIX A**

In this appendix, we compute $\mathbb{E}(B^n_0)^2$, $\mathbb{E}(B^0_0)^2$, and $\mathbb{E}(B^n_0 B^0_0)$. We begin with the last expression. We have

$$\mathbb{E}(B^n_0 B^0_0) = \sum_{k=1}^{\infty} \Lambda_k(u)\Lambda_k(\tau)$$

$$= \int_0^u \int_0^\tau \sum_{k=1}^{\infty} \lambda_k(u')\lambda_k(\tau')d\tau' du'$$

$$= \int_0^u \int_0^\tau [\delta(u' - \tau') - 1] d\tau' du'$$

where we used the completeness relation. In this sense, the reader should remember that $\{\lambda_k(u)\}_{k \geq 1}$ together with the constant function make up a complete basis in $L^2([0, 1])$. Now, let $I_u(u')$ and $I_\tau(\tau')$ denote the indicator functions of the intervals $[0, u]$ and $[0, \tau]$, respectively. The last integral in Eq. (A1) becomes

$$\mathbb{E}(B^n_0 B^0_0) = \int_0^1 \int_0^1 I_u(u') I_\tau(\tau') \delta(u' - \tau') d\tau' du' - u\tau$$

$$= \int_0^1 I_u(u') I_\tau(u') du' - u\tau = \min(u, \tau) - u\tau. \quad (A2)$$

Then, the expressions for $\mathbb{E}(B^n_0)^2$ and $\mathbb{E}(B^0_0)^2$ are readily obtained by setting $u = \tau$ in (A2). We notice that the above expectations are independent of the particular random series representation of the Brownian bridge, as they should be.

**APPENDIX B**

In this appendix, we prove that for the Wiener-Fourier series we have

$$\lim_{n \to \infty} \frac{\int_0^1 \int_0^1 \gamma_n(u, \tau) h(u, \tau) dud\tau}{\int_0^1 \int_0^1 \gamma_n(u, \tau) dud\tau} = \int_0^1 h(u, u) du \quad (B1)$$

for all continuous functions $h(u, \tau)$. This is the statement of Eq. (13) in Section II.B. We start with the equations

$$\gamma_n(u, \tau) = \frac{2}{\pi^2} \sum_{k=n+1}^{\infty} \frac{\sin(k\pi u)\sin(k\pi \tau)}{k^2} \quad (B2)$$

and

$$\int_0^1 \int_0^1 \gamma_n(u, \tau) dud\tau = \frac{1}{\pi^2} \sum_{k=n+1}^{\infty} \frac{1}{k^2}.$$ 

By letting $n \to \infty$ in the sequence of inequalities

$$\frac{1}{3} \frac{n^3}{(n+1)^3} = n^3 \int_0^1 x^{-4} dx \leq \sum_{k=n+1}^{\infty} n^3/k^4$$

$$\leq n^3 \int_0^1 x^{-4} dx = \frac{1}{3}, \quad (B3)$$

one deduces that

$$\lim_{n \to \infty} \int_0^1 \int_0^1 \gamma_n(u, \tau) dud\tau = \frac{1}{3\pi^2}. \quad (B4)$$

Therefore, Eq. (B1) can be reformulated as

$$3\pi^4 \lim_{n \to \infty} n^3 \int_0^1 \int_0^1 \gamma_n(u, \tau) h(u, \tau) dud\tau = \int_0^1 h(u, u) du \quad (B5)$$

We prove the relation (B5) in two steps. The first step is to set $h(u, \tau) = |h(u, \tau) - h(u, u)|$ and show that

$$3\pi^4 \lim_{n \to \infty} n^3 \int_0^1 \int_0^1 \gamma_n(u, \tau) h(u, \tau) dud\tau = 0. \quad (B6)$$

For that purpose, pick an arbitrary $\eta > 0$. Let us notice that $h(u, \tau)$ is continuous on the compact set $[0, 1] \times [0, 1]$, thus bounded by a constant $M < \infty$ and uniformly continuous. The second property implies that there is $1 > \epsilon > 0$ such that $|h(u', \tau') - h(u, \tau)| < \eta$ whenever $(u' - u)^2 + (\tau' - \tau)^2 < \epsilon^2$. Now, notice that by construction $h(u, u) = 0$ for all $0 \leq u \leq 1$. Since any point $(u, \tau)$ in the set

$I_\epsilon = \{(u, \tau) \in [0, 1] \times [0, 1] : |u - \tau| < \epsilon\}$ 

is contained in the ball of radius \( \epsilon \) centered about the point \((u, u)\), by uniform continuity, it follows that \( h'(u, \tau) < \eta \) on \( I_r \).

Let us break the integral in Eq. (B6) in two parts: one over the set \( I_r \) and the other on its complementary \( I_r^c = [0, 1] \times [0, 1] - I_r \). For the integral over the set \( I_r \) we have

\[
3\pi^4 \limsup_{n \to \infty} n^3 \int_{I_r} \gamma_n(u, \tau)^2 h'(u, \tau) d\tau \leq \eta \left[ 3\pi^4 \limsup_{n \to \infty} n^3 \int_{I_r} \gamma_n(u, \tau)^2 d\tau \right] \leq \eta. \tag{B7}
\]

For the integral over the set \( I_r^c \), we have the estimate

\[
3\pi^4 \limsup_{n \to \infty} n^3 \int_{I_r^c} \gamma_n(u, \tau)^2 h'(u, \tau) d\tau \leq M \left[ 3\pi^4 \limsup_{n \to \infty} n^3 \int_{I_r^c} \gamma_n(u, \tau)^2 d\tau \right]. \tag{B8}
\]

We intend to show that the last limit in Eq. (B8) is zero and for this purpose, we need to construct a sharp bound of the function \( \gamma_n(u, \tau) \) on the set \( I_r^c \). It turns out that we first need to study the behavior of the functions

\[
\sum_{k=n+1}^{\infty} \frac{\cos(k\pi u)}{k^2}
\]

on the interval \((0, 2)\).

We have

\[
sin(\pi u/2) \sum_{k=n+1}^{\infty} \frac{\cos(k\pi u)}{k^2} = \frac{1}{2} \sum_{k=n+1}^{\infty} \frac{\sin((k+1/2)\pi u)}{k^2} \leq \frac{1}{2} \sum_{k=n+1}^{\infty} \frac{\sin((k+1/2)\pi u)}{(n+1)^2}, \tag{B9}
\]

\[
+ \frac{1}{2} \sum_{k=n+1}^{\infty} \frac{1}{(k+1)^2} \sin([k+1/2]\pi u).
\]

From Eq. (B9) we learn that

\[
\sin(\pi u/2) \left| \sum_{k=n+1}^{\infty} \frac{\cos(k\pi u)}{k^2} \right| \leq \frac{1}{2(n+1)^2}
\]

\[
+ \frac{1}{2} \sum_{k=n+1}^{\infty} \left[ \frac{1}{k^2} - \frac{1}{(k+1)^2} \right] \sin((k+1/2)\pi u).
\]

Therefore,

\[
\left| \sum_{k=n+1}^{\infty} \frac{\cos(k\pi u)}{k^2} \right| \leq \frac{1}{(n+1)^2} F(u), \tag{B10}
\]

where the function

\[
F(u) = \frac{1}{\sin(\pi u/2)}
\]

is continuous on the interval \((0, 2)\), decreasing on the interval \((0, 1]\) and increasing on the interval \([1, 2)\).

Using the bound given by Eq. (B10), together with the inequality \((a - b)^2 \leq 2(a^2 + b^2)\), one computes

\[
\gamma_n(u, \tau)^2 = \frac{1}{\pi^4} \left\{ \sum_{k=n+1}^{\infty} \frac{\cos(k\pi(u - \tau)) - \cos(k\pi(u + \tau))}{k^2} \right\}^2
\]

\[
\leq \frac{2}{\pi^4} \left\{ \left[ \sum_{k=n+1}^{\infty} \frac{\cos(k\pi|u - \tau|)}{k^2} \right]^2 + \left[ \sum_{k=n+1}^{\infty} \frac{\cos(k\pi|u + \tau|)}{k^2} \right]^2 \right\}
\]

\[
\leq \frac{2}{\pi^4(n+1)^4} \left[ F(|u - \tau|)^2 + F(|u + \tau|)^2 \right]. \tag{B12}
\]

On the set \( I_r^c \), we have \( \epsilon \leq |u - \tau| \leq 1 \) and \( \epsilon \leq |u + \tau| \leq 2 - \epsilon \). Therefore, \( F(|u - \tau|) \leq F(\epsilon) \) and \( F(|u + \tau|) \leq F(\epsilon) \).

Corroborating with Eq. (B12), we obtain

\[
\gamma_n(u, \tau)^2 \leq \frac{4}{\pi^4(n+1)^4} F(\epsilon)^2 \quad \text{if} \ (u, \tau) \in I_r^c. \tag{B13}
\]
Replacing the estimate (B13) in Eq. (B8), one readily concludes that the limit in Eq. (B8) is 0. Adding the limits of Eq. (B7) and Eq. (B5), we conclude that

$$3\pi^4 \lim_{n \to \infty} n^3 \int_0^1 \int_0^1 \gamma_n(u, \tau)^2 h(u, \tau) \, du \, d\tau \leq \eta.$$  \hspace{1cm} (B14)

Since $\eta > 0$ is arbitrary, the equality (B5) is demonstrated.

In the second step of the proof, we show that Eq. (B6) implies the relation (B1). From Eq. (B6), one deduces that

$$3\pi^4 \lim_{n \to \infty} n^3 \int_0^1 \int_0^1 \gamma_n(u, \tau)^2 h(u, \tau) \, du \, d\tau = 3\pi^4 \lim_{n \to \infty} n^3 \int_0^1 \int_0^1 \gamma_n(u, \tau)^2 h(u, \tau) \, du \, d\tau. \hspace{1cm} (B15)$$

By explicitly computing the integral over $\tau$, the last relation becomes

$$3\pi^4 \lim_{n \to \infty} n^3 \int_0^1 f_n(u) h(u, u) \, du, \hspace{1cm} (B16)$$

where

$$f_n(u) = \frac{2}{\pi^4} \sum_{k=n+1}^{\infty} \frac{\sin(k\pi u)^2}{k^4} = \frac{1}{\pi^4} \sum_{k=n+1}^{\infty} \frac{1 - \cos(2k\pi u)}{k^4}. \hspace{1cm} (B17)$$

By continuity, $h(u, u)$ is integrable and if we set

$$B_k = \int_0^1 \cos(2k\pi u) h(u, u) \, du,$$

the Riemann-Lebesgue lemma says that

$$\lim_{n \to \infty} |B_k| = \limsup_{n \to \infty} |B_k| = 0.$$  \hspace{1cm} (B18)

We notice that

$$3\pi^4 \lim_{n \to \infty} \frac{n^3}{\pi^4} \sum_{k=n+1}^{\infty} \int_0^1 \frac{\cos(2k\pi u)}{k^4} h(u, u) \, du \leq 3\pi^4 \lim_{n \to \infty} \left[ \frac{n^3}{\pi^4} \left( \sum_{k=n+1}^{\infty} \frac{1}{k^4} \right) \sup_{k \geq n+1} |B_k| \right] \leq \lim_{n \to \infty} \sup_{k \geq n+1} |B_k| = 0.$$  \hspace{1cm} (B19)

Therefore, the terms containing $\cos(2k\pi u)$ in the Eq. (B17) may be dropped and the quantity (B15) becomes

$$3\pi^4 \lim_{n \to \infty} \frac{n^3}{\pi^4} \left( \sum_{k=n+1}^{\infty} \frac{1}{k^4} \right) \int_0^1 h(u, u) \, du = \int_0^1 h(u, u) \, du, \hspace{1cm} (B18)$$

where we used (B4) to compute the last limit. The relation (B1) is therefore proved.

**APPENDIX C**

It is well known that if $A,B > 0$, and $\alpha = C/\sqrt{AB}$ such that $|\alpha| < 1$, then the following Mehler's formula holds for all $f$ and $g$ whose squares have finite Gaussian transforms

$$|f \circ g|_{ABC}(x_0, y_0) = \left\{ \int_R \int_R \frac{1}{2\pi \sqrt{AB - C^2}} \exp \left( -\frac{1}{2} \frac{x^2B + y^2A - 2xyC}{AB - C^2} \right) f(x_0 + x)g(y_0 + y) \right\} \left( \int_R \int_R \frac{1}{2\pi \sqrt{1 - \alpha^2}} \exp \left( -\frac{1}{2} \frac{x^2 + y^2 - 2xy\alpha}{1 - \alpha^2} \right) f(x_0 + x\sqrt{A})g(y_0 + y\sqrt{B}) \right)^2 \hspace{1cm} (C1)$$

In the above, the functions $H_k(x)$ are the normalized Hermite polynomials corresponding to the Gaussian weight

$$d\mu(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}.$$  \hspace{1cm} (C1)

They form a complete orthonormal basis in the Hilbert space $L_2^2(\mathbb{R})$, which is endowed with the scalar product

$$\langle \psi| \phi \rangle = \int_R \psi(x)\phi(x) \, d\mu(x).$$

Let us notice that according to our hypothesis, the functions $f(x_0 + x\sqrt{A})$ and $g(y_0 + y\sqrt{B})$ as functions of $x$ are square integrable against $d\mu(x)$ and thus they lie in the Hilbert space $L_2^2(\mathbb{R})$.

By repeated integration by parts, the formula (C1) is shown to equal

$$|f \circ g|_{ABC}(x_0, y_0) = \sum_{k=0}^{\infty} \frac{C^k}{k!} f_{A}^{(k)}(x_0) g_{B}^{(k)}(y_0), \hspace{1cm} (C2)$$
where in general \( f^{(k)}(x_0) \) is the \( k \)-order derivative of 
\[ f_A(x_0) = \int_{\mathbb{R}} \frac{1}{\sqrt{2\pi A}} e^{-z^2/(2A)} f(x_0 + z) dz. \]

Let us notice that the series (C1) can be extended to the case \( \alpha = 1 \), too. Indeed, the last series in Eq. (C1) for the case \( \alpha = 1 \) is nothing else but the Bessel series 
\[ \sum_{k=0}^{\infty} \langle H_k | f(x_0 + \sqrt{A}) \rangle \langle H_k | g(y_0 + \sqrt{B}) \rangle, \]
which is convergent to 
\[ \left( f(x_0 + \sqrt{A}) \right) \left( g(y_0 + \sqrt{B}) \right) \]
\[ = \int_{\mathbb{R}} f(x_0 + x \sqrt{A}) g(y_0 + x \sqrt{B}) d\mu(x). \]

Next, we proceed to establish the relation (C3). We start with the identity 
\[ E_n \left[ U_{\infty}(x, x', \beta; \bar{\alpha}) - U_{\infty}(x, x', \beta; \bar{\alpha}) \right]^2 = E_n \left[ U_{\infty}(x, x', \beta; \bar{\alpha}) - U_{\infty}(x, x', \beta; \bar{\alpha}) \right]^2 \quad \text{(C3)} \]
Using the notation introduced in Section II.A, we have 
\[ E_n U_{\infty}(x, x', \beta; \bar{\alpha}) = \nabla_{u,n}[x_r(u) + \sigma S_n^u(\bar{\alpha})]. \quad \text{(C4)} \]
Moreover, 
\[ E_n U_{\infty}(x, x', \beta; \bar{\alpha}) = \int_{0}^{1} du \int_{0}^{u} d\tau E_n V[x_r(u) + \sigma S_n^u(\bar{\alpha}) + \sigma B_n^u(\bar{\alpha})]V[x_r(\tau) + \sigma S_n^r(\bar{\alpha}) + \sigma B_n^r(\bar{\alpha})] \quad \text{(C5)} \]
and remembering that the variables \( B_n^u(\bar{\alpha}) \) and \( B_n^r(\bar{\alpha}) \) have a joint Gaussian distribution of covariances given by Eq. (7), we obtain 
\[ E_n U_{\infty}(x, x', \beta; \bar{\alpha})^2 = \int_{0}^{1} du \int_{0}^{u} d\tau \int_{\mathbb{R}} dx \int_{\mathbb{R}} dy \frac{1}{2\pi \Delta_n(u, \tau)} \]
\[ \begin{vmatrix} 1 - x^2 \Gamma_n^2(\tau) + y^2 \Gamma_n^2(u) - 2xyG_n(u, \tau) \end{vmatrix} \]
\[ \times V[x_r(u) + \sigma S_n^u(\bar{\alpha}) + x]V[x_r(\tau) + \sigma S_n^r(\bar{\alpha}) + y], \]
where \( G_n(u, \tau) = \sigma^2 \gamma_n(u, \tau) \) and 
\[ \Delta_n^2(u, \tau) = \Gamma_n^2(u) \Gamma_n^2(\tau) - G_n(u, \tau)^2. \]

Using the expansion (C2), one may write the above integral as the sum of the series 
\[ E_n U_{\infty}(x, x', \beta; \bar{\alpha})^2 = \sum_{k=0}^{\infty} \frac{1}{k!} \int_{0}^{1} du \int_{0}^{u} d\tau G_n(u, \tau)^k \times \left( \nabla_{u,n}^{(k)}[x_r(u) + \sigma S_n^u(\bar{\alpha})] \nabla_{r,n}^{(k)}[x_r(\tau) + \sigma S_n^r(\bar{\alpha})] \right), \]
where \( \nabla_{u,n}^{(k)}(x) \) is the \( k \)-order derivative of \( \nabla_{u,n}(x) \). With the help of Eq. (C1), one recognizes the first term of the above series to be \( [E_n U_{\infty}(x, x', \beta; \bar{\alpha})]^2 \), so that Eq. (C3) becomes 
\[ E_n \left[ U_{\infty}(x, x', \beta; \bar{\alpha}) - U_{\infty}(x, x', \beta; \bar{\alpha}) \right]^2 = \sum_{k=1}^{\infty} \frac{1}{k!} \int_{0}^{1} du \int_{0}^{u} d\tau G_n(u, \tau)^k \times \nabla_{u,n}^{(k)}[x_r(u) + \sigma S_n^u(\bar{\alpha})] \nabla_{r,n}^{(k)}[x_r(\tau) + \sigma S_n^r(\bar{\alpha})]. \quad \text{(C6)} \]
As mentioned in Section II.B, the kernels \( \gamma_n(u, \tau) \) and therefore \( G_n(u, \tau) \) are positive definite for all integers \( k \geq 1 \) so that the terms of the series (C6) are all positive i.e., 
\[ \int_{0}^{1} du \int_{0}^{u} d\tau G_n(u, \tau)^k \nabla_{u,n}^{(k)}[x_r(u) + \sigma S_n^u(\bar{\alpha})] \nabla_{r,n}^{(k)}[x_r(\tau) + \sigma S_n^r(\bar{\alpha})] \geq 0 \]
for all \( k \geq 1 \). Because of this property, the series (C6) will plays the fundamental role in establishing the various results in this appendix. Truncating the series (C6) to the first term, we obtain the inequality 
\[ E_n \left[ U_{\infty}(x, x', \beta; \bar{\alpha}) - U_{\infty}(x, x', \beta; \bar{\alpha}) \right]^2 \geq E_n T_n'(x, x', \beta; \bar{\alpha}), \quad \text{(C7)} \]
where 
\[ T_n'(x, x', \beta; \bar{\alpha}) = \int_{0}^{1} du \int_{0}^{u} d\tau G_n(u, \tau) \times \nabla_{u,n}^{(1)}[x_r(u) + \sigma S_n^u(\bar{\alpha})] \nabla_{r,n}^{(1)}[x_r(\tau) + \sigma S_n^r(\bar{\alpha})]. \]
In a similar fashion, if we truncate the series (C6) to the first two terms, we obtain 
\[ E_n \left[ U_{\infty}(x, x', \beta; \bar{\alpha}) - U_{\infty}(x, x', \beta; \bar{\alpha}) \right]^2 \geq E_n Y_n'(x, x', \beta; \bar{\alpha}), \quad \text{(C8)} \]
where 
\[ Y_n'(x, x', \beta; \bar{\alpha}) = T_n'(x, x', \beta; \bar{\alpha}) + \frac{1}{2} \int_{0}^{u} du \int_{0}^{u} d\tau G_n(u, \tau)^2 \times \nabla_{u,n}^{(2)}[x_r(u) + \sigma S_n^u(\bar{\alpha})] \nabla_{r,n}^{(2)}[x_r(\tau) + \sigma S_n^r(\bar{\alpha})]. \]
Now, we assume that \( V(x) \in \cap_\alpha W^{1,2}(\mathbb{R}) \). The inequality \( 1/k! \leq 1/(k - 1)! \) and the positivity of the terms of the series (C6) imply
The equation (C13) can be deduced by remembering that the Brownian bridges $B_{u,k}^0$ for each dimension are independent processes. Then, one successively applies the
expansion (C6) for each dimension to obtain Eq. (C13).

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