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Applying reproducing kernels to the evaluation and approximation of the simple and time-dependent imaginary time harmonic oscillator path integrals

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Reproduction of kernel Hilbert spaces offers an attractive setting for imaginary time path integrals, since they allow to naturally define a probability on the space of paths, which is equal to the probability associated with the paths in Feynman's path integral formulation. This study shows that if the propagator is Gaussian, its variance equals the squared norm of a linear functional on the space of paths. This can be used to rederive the harmonic oscillator propagator, as well as to offer a finite-dimensional perturbative approximation scheme for the time-dependent oscillator wave function and its ground state energy, and its bound error. The error is related to the rate of decay of the Fourier coefficients of the time-dependent part of the potential. When the rate of decay increases beyond a certain threshold, the error in the approximation over a subspace of dimension n is of order $(1/n^3)$.

Keywords: Path integral; Imaginary time; Finite-dimensional approximation; Reproducing kernels; Time-dependent harmonic oscillator

Mathematics Subject Classifications: Numerical analysis 65Z05 (applications to physics); General mathematical topics and methods in quantum theory 81Q30 (Feynman integrals)

1. Introduction

In the path integral formulation of quantum mechanics [1–3], the propagator $U(x_1, T_1; x_0, T_0)$ is expressed as the integral of $\exp(iS[x(t)])$ (assume $\hbar = 1$) over all paths $x(t)$ satisfying $x(T_0) = x_0$, $x(T_1) = x_1$, where $S[x(t)]$ is the classical action along the path. In the so-called imaginary time formulation, this oscillatory integral

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is replaced by the integral of $\exp(-S[x(t)])$, with the potential reversed. This is a Gaussian integral which has nicer convergence properties (often, imaginary time is denoted by τ to distinguish it from real time t, but here only imaginary time is used and it is denoted by t).

It is immediate that if the wave function at $t=0$, $\psi(0)$, is the delta function $\delta(x)$, then $U(x,T;0,0)$ equals $\psi(T)$ the wave function at time T. For simplicity, the discussion is limited to the initial condition $\psi(0)=\delta(x)$ unless otherwise stated.

The probability distribution on the paths $x(t)$ induces a distribution on the value at the paths' endpoints, $x(T)$. The probability density f on the space of paths is defined in imaginary time formulation by

$$f[x(t)] \propto \exp(-S[x(t)]) \tag{1}$$

(note that in imaginary time there is no phase, hence the difference between amplitude and probability is just a factor of two in the exponent). This probability naturally induces a probability distribution on the values of the paths at time T, and it is this distribution which defines $\psi(T)$. One can thus, for example, define the expectation and variance respectively of $\psi(T)$ by

$$E_T \equiv \int_{x(t)} x(T)\exp(-S[x(t)])Dx(t), \quad V_T \equiv \int_{x(t)} [x(T)-E_T]^2\exp(-S[x(t)])Dx(t)$$

where the integral is over the Sobolev space of paths satisfying $x(0)=0$ and such that $x'(t)$ is square integrable on $[0,T]$. The condition $x(0)=0$ corresponds to the condition $\psi(0)=\delta(x)$.

Such integrals can be computed, even though the path space is infinite-dimensional, using the theory of reproducing kernels [4] and Gaussian measures, some of which is summarized in [5]. The result required in this work is the following: if (x,y) is an inner product on a Hilbert space Ω, and $v_0 \in \Omega$, then a measure can be defined such that $\int_\Omega \exp(-\|x\|^2)Dx = 1$ and

$$\int_\Omega \|(v_0,x)\|^2 \exp\left(-\|x\|^2\right)Dx = \frac{\|v_0\|^2}{2}$$

and further, $x \to (v_0,x)$ defines a Gaussian random variable on Ω, with zero average and a variance of $(1/2)\|v_0\|^2$. This is a natural extension of the finite-dimensional Gaussian integral. In order to apply this result to compute $\psi(T)$, one needs to define an appropriate inner product on the space of paths (which corresponds to the action), and also to write $x(T)$ as an inner product with a certain vector in the space of paths (naturally, this vector is also a path). This is achieved, for example, by using the inner product

$$(x,y) = \left(\frac{m}{2}\right)\int_0^T \left[x'(t)y'(t)+\omega^2 x(t)y(t)\right]\mathrm{dt} \tag{2}$$

for the simple harmonic oscillator, and

$$(x, y) = \left(\frac{m}{2}\right) \int_0^T [x'(t)y'(t) + \omega(t)x(t)y(t)]\mathrm{d}t \tag{2'}$$

for the time dependent oscillator (assume $\omega(t) \geq 0$). It is immediate to verify that in both cases, $S[x(t)] = \|x(t)\|^2$. Thus the main effort is to find the *reproducing kernel* e_T which satisfies $(x, e_T) = x(T)$ for every path $x(t)$, that is, e_T is the reproducing kernel for the *evaluation at* T functional (which will usually be referred to simply as 'the evaluation at T'). Once e_T is known, then the variance of $\psi(T)$ can easily be computed using the identity $\mathrm{Var}[\psi(T)] = (1/2)\|e_T\|^2 = (1/2)e_T(T)$, where the last equality follows from the definition of e_T as a reproducing kernel.

Note that as opposed to most of the methods which integrate over paths tied at the two endpoints (i.e., satisfying $x(T_0) = x_0,\ x(T_1) = x_1$), here the integration is carried over paths tied only at $t = 0$.

Note that one may look at the problem of estimating $x(T)$ as a problem of *Bayesian estimation*, in which $x(0)$ is known (the measurement data), and a *prior probability* is given over the paths $x(t)$, which assigns lower probability to 'rougher' paths. Given the data and the prior, $x(T)$ can be estimated. However, this direction is not be pursued here.

As observed before, under the probability structure of equation (1), $x \to x(T)$ is a Gaussian random variable. This means that $\psi(T)$ is a Gaussian; hence it is fully determined not only by its expectation and variance but also by a multiplicative constant. In [5], the probability on the entire space is normalized to one; however, from physical considerations, $\psi(T)$ should be normalized with respect to the free particle wave function, i.e., multiplied by what may be loosely termed the 'probability reduction factor':

$$P_{rf} = \frac{\int_{x(t)} \exp(-S[x(t)])Dx(t)}{\int_{x(t)} \exp(-S_F[x(t)])Dx(t)} \tag{3}$$

where S_F is the free particle action (see [6]). Thus calculating/approximating the wave function is equivalent to calculating/approximating the norm of e_T, as well as P_{rf}. As for the expectation, if $x(0) = 0$, it is clearly zero from symmetry considerations; the general case is quite similar and is treated in Appendix I.

1.1 *Reproducing kernels and finite-dimensional approximations*

How to calculate the reproducing kernel's norm? The norm squared of e_T equals $e_T(T)$. Usually, however, e_T cannot be calculated exactly. The norm squared of e_T also equals $\sup \int_{x(t)} (x^2(T))/(\|x\|^2)$, which, for the time-dependent oscillator, for example, is

$$\sup_{x(t)} \frac{x^2(T)}{\|x\|^2} = \sup_{x(t)} \frac{x^2(T)}{(m/2)\int_0^T \left[x'(t)^2 + \omega(t)x^2(t)\right]\mathrm{d}t} \tag{4}$$

where the supremum is taken over the aforementioned Sobolev space of paths. Note that any choice of $x(t)$ defines a lower bound on the norm (and thus on the variance, or the spread, of the wave function). A clever choice of $x(t)$ can thus yield a good lower bound.

Although normally the expression in equation (4) cannot be evaluated exactly, the representation as the norm of a linear functional can still be useful for choosing good finite-dimensional approximations to the path integral: suppose that V is the entire space and F a finite-dimensional subspace. Intuitively, for the norm restricted to F to be a good approximation to the norm on V, it is desirable that, if $\bar{F}$ is the complement of F, then $x^2(T)$ will be relatively small and $\int_0^T [x'(t)^2 + \omega(t)x^2(t)]\mathrm{d}t$ relatively large for $x(t) \in \bar{F}$. Intuitively, that will ensure that the norm on F's complement will be small. A solution which is sought in this study is to construct an increasing sequence of subspaces $\{F_n\}$ ($F_{n+1} \supset F_n$ for every n) such that $\cup_n F_n = V$, and if $F_{n+1} = \mathrm{span}(F_n \cup f_{n+1})$, then the norm of the functional $x \to x(T)$ on the 'supplement' f_{n+1} is small or, equivalently,

$$\frac{f_{n+1}^2(T)}{\int_0^T \left[f'_{n+1}(t)^2 + \omega(t) f_{n+1}^2(t)\right]\mathrm{d}t}$$

is small. If the norm restricted to $\mathrm{span}(f_{n+1})$ decreases quickly enough with n, there is hope that the norm on F_k, for a relatively small k, will be a good approximation to the norm on the entire space V. Similar considerations apply to the approximation of P_{rf} on finite-dimensional subspaces.

1.2 *Structure of this article*

In section 2, the framework for computing the propagator is summarized. Section 3 shows how the free particle and simple harmonic oscillator propagators can be computed using the reproducing kernel approach; it is also shown how the uncertainty associated with a quantum particle's velocity can be computed very naturally in the reproducing kernel framework. Section 4 discusses bounds on the accuracy of finite-dimensional approximations for the propagator of the time-dependent harmonic oscillator. Section 5 offers some concluding remarks. Appendix I treats the propagator for an arbitrary starting point, and Appendix II relates the ground state energy to the 'probability reduction factor'.

2. General scheme for computing or approximating the wave function and ground state energy

The suggested method for computing or approximating the wave function $\psi(T)$ may be summarized thusly:

- Write down the action as an inner product in the appropriate Sobolev space of paths $x(t)$. The inner product must satisfy $S[x(t)] = \|x(t)\|^2$.
- Compute the reproducing kernel for the evaluation functional at T, i.e., a function e_T satisfying $(x, e_T) = x(T)$ for every path $x(t)$.
- The variance of $\psi(T)$ is $V_T = (1/2)e_T(T)$.

- Compute the 'probability reduction factor'

$$P_{rf} = \frac{\int_{x(t)} \exp(-S[x(t)])Dx(t)}{\int_{x(t)} \exp(-S_F[x(t)])Dx(t)},$$

  where $S_F[x(t)] = (m/2)\int_0^T x'(t)^2 \mathrm{d}t$ is the free particle action.
- $\psi(T)$ equals $P_{rf}/(\sqrt{2\pi V_T})\exp(-(x^2/2V_T))$.
- Usually, V_T and P_{rf} cannot be calculated exactly. In that case, seek an increasing sequence of subspaces F_n whose union is the entire space of paths, such that the ratio of the value of V_T resp. P_{rf} when restricted to F_{n+1} over the value when restricted to F_n quickly tends to 1. Then the values on the entire space can be approximated using the values on a finite-dimensional subspace and asymptotic analysis.
- The ground state energy is closely related to P_{rf} (Appendix II), hence it can be approximated by the same scheme used to approximate P_{rf}.

3. Derivation of the free particle and harmonic oscillator propagators

3.1 *Free particle propagator*

For the free particle, the probability associated with the path $x(t)$ is $\exp(-(m/2)\int_0^T x'(t)^2 \mathrm{d}t)$, hence the inner product in the Sobolev space is simply $(x, y) = (m/2)\int_0^T x'(t)y'(t)\mathrm{d}t$. The reproducing kernel e_T must then satisfy $(x, e_T) = x(T)$ for every path $x(t)$ such that $x(0) = 0$. Also, it must hold that $e_T(0) = 0$. It is straightforward to see that $e_T(t) = (2/m)t$, hence $(1/2)e_T(T) = (T/m)$. From the aforementioned results on Gaussian integrals, the free particle propagator is a Gaussian with variance (T/m), and if it is further demanded that it will be normalized to 1, it must equal $(m/2\pi T)^{1/2}\exp(-(m/2T)x^2)$.

3.2 *Simple harmonic oscillator propagator*

The inner product corresponding to the simple harmonic oscillator was defined in equation (2). To distinguish it from the free particle inner product, denote it by $(x, y)_O = (m/2)\int_0^T \left[x'(t)y'(t) + \omega^2 x(t)y(t)\right]\mathrm{d}t$. The inner product corresponding to the free particle will be denoted $(x, y)_F = (m/2)\int_0^T x'(t)y'(t)\mathrm{d}t$. Next, recover the reproducing kernel e_T satisfying $(x, e_T)_O = x(T)$ for all paths x. This can be done by expanding e_T in a basis $\{\beta_l\}$ for the Sobolev space, and determining the coefficients by imposing the condition $(\beta_l, e_T) = \beta_l(T)$ for every l. Choosing the basis $\beta_0 = t$, $\beta_1 = \sin(\pi/T)$, $\beta_2 = \sin(2\pi/T)\ldots$ (note that it is indeed a basis because the paths satisfy $x(0) = 0$; this basis is nearly the same as that used in the Fourier path integral method [4]), denote $e_T(t) = \sum_{l=0}^{\infty}\alpha_l\beta_l$. Next, obtain the following equations for $\{\alpha_l\}$: first, impose $(\beta_0, e_T) = \beta_0(T)$ to obtain

$$T = t(T) = (t, e_T)_O = \alpha_0(t, t)_O + \sum_{l=1}^{\infty}\alpha_l\left(\sin\left(\frac{l\pi t}{T}\right), t\right)_O \equiv \alpha_0 t_t + \sum_{l=1}^{\infty}\alpha_l t_l \tag{5}$$

$$t_t = (\beta_0, \beta_0)_O = (t, t)_O = \frac{1}{2}mT + \frac{1}{6}m\omega^2 T^3, \quad l > 0 \Rightarrow t_l = (\beta_0, \beta_l)_O = \left(t, \sin\left(\frac{l\pi t}{T}\right)\right)_O$$
$$= \frac{(-1)^{k+1}m\omega^2 T^2}{2\pi l} \tag{5'}$$

and for $l > 0$ impose $(\beta_l, e_T) = \beta_l(T)$ to obtain

$$0 = \sin\left(\frac{l\pi t}{T}\right)(T) = \left(\sin\left(\frac{l\pi t}{T}\right), e_T\right)_O = \alpha_0\left(\sin\left(\frac{l\pi t}{T}\right), t\right)_O + \sum_{k=1}^{\infty}\alpha_k\left(\sin\left(\frac{l\pi t}{T}\right), \sin\left(\frac{k\pi t}{T}\right)\right)_O \equiv \alpha_0 t_l + \alpha_l l_l \tag{5''}$$

where

$$l_l = (\beta_l, \beta_l)_O = \left(\sin\left(\frac{l\pi t}{T}\right), \sin\left(\frac{l\pi t}{T}\right)\right)_O = \frac{m\left(\omega^2 T^2 + \pi^2 l^2\right)}{4T}$$

(in 5″use $k \neq l \Rightarrow (\sin(l\pi t/T), \sin(k\pi t/T))_O = 0$).

From (5″) it follows that for $l > 0$, $\alpha_l = -(t_l/l_l)\alpha_0$. Plugging this into (5) yields

$$T = \alpha_0 t_t - \sum_{l=1}^{\infty}\frac{t_l^2}{l_l}\alpha_0, \quad \text{so} \quad \alpha_0 = \frac{T}{t_t - \sum_{l=1}^{\infty}(t_l^2/l_l)}.$$

Note that since $l > 0 \Rightarrow \beta_l(T) = 0$, then

$$e_T(T) = \alpha_0 T = \frac{T^2}{t_t - \sum_{l=1}^{\infty}(t_l^2/l_l)}.$$

This expression can be evaluated by summing the infinite series $\sum_{l=1}^{\infty}(t_l^2/l_l)$, which, up to a constant factor, equals

$$\sum_{l=1}^{\infty}\frac{1}{l^2(\omega^2 T^2 + \pi^2 l^2)}. \tag{5'''}$$

Sparing the details, the result for the variance turns out to be

$$V_T = \frac{1}{2}e_T(T) = \frac{1}{m\omega\coth(\omega T)}.$$

Note that if the computation was restricted to the subspace spanned by $\{\beta_0, \beta_1, \ldots, \beta_{n-1}\}$, the error in equation (5‴) – and in the overall expression for V_T as well – would have been of the order of $(1/n^3)$. Under certain conditions, this is also the error bound for the time-dependent oscillator (section 4).

Next, the 'probability reduction factor' is computed. Denote as before $\{\beta_0 = t, \beta_1 = \sin(\pi t/T), \beta_2 = \sin(2\pi t/T), \ldots,\}$, and let $V_n = \text{span}\{\beta_0, \beta_1, \ldots, \beta_{n-1}\}$. Then, from equation (3) and using the well-known results on Gaussian integrals,

$$P_{rf} = \frac{\int_{x(t)}\exp(-S_O[x(t)])Dx(t)}{\int_{x(t)}\exp(-S_F[x(t)])Dx(t)} = \lim_{n\to\infty}\int\frac{\int_{V_n}\exp(-S_O[x(t)])Dx(t)}{\int_{V_n}\exp(-S_F[x(t)])Dx(t)} = \lim_{n\to\infty}\int\sqrt{\frac{\left|G_F^{(n)}\right|}{\left|G_O^{(n)}\right|}} \tag{6}$$

where S_O resp. S_F are the oscillator resp. free particle actions, and $G_O^{(n)}, G_F^{(n)}$ are $n \times n$ matrices (Grammians) defined by

$$\left[G_O^{(n)}\right]_{k,l} = (\beta_k, \beta_l)_O, \ \left[G_F^{(n)}\right]_{k,l} = (\beta_k, \beta_l)_F \quad \text{for } 0 \le k, \ l \le n-1.$$

It is easy to see that $G_F^{(n)}$ is diagonal with

$$\left[G_F^{(n)}\right]_{0,0} = \frac{mT}{2}$$

and for $l > 0$,

$$\left[G_F^{(n)}\right]_{l,l} = \frac{m\pi^2 l^2}{4T},$$

thus

$$\left|G_F^{(n)}\right| = (mT/2) \prod_{k=1}^{n-1} \frac{m\pi^2 k^2}{4T}.$$

$G_O^{(n)}$ is 'nearly diagonal': using the notations from equations (5 to 5‴),

$$\left[G_O^{(n)}\right]_{k,l} = (\beta_k, \beta_l)_O,$$

so it can be diagonalized by the process outlined below:

$$G_O^{(n)} = \begin{pmatrix} t_t & t_1 & t_2 & t_3 & \cdots \\ t_1 & l_1 & 0 & 0 & \cdots \\ t_2 & 0 & l_2 & 0 & \cdots \\ t_3 & 0 & 0 & l_3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \to \begin{pmatrix} t_t - \frac{t_1^2}{l_1} & 0 & t_2 & t_3 & \cdots \\ t_1 & l_1 & 0 & 0 & \cdots \\ t_2 & 0 & l_2 & 0 & \cdots \\ t_3 & 0 & 0 & l_3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$\to \begin{pmatrix} t_t - \frac{t_1^2}{l_1} - \frac{t_2^2}{l_2} & 0 & 0 & t_3 & \cdots \\ t_1 & l_1 & 0 & 0 & \cdots \\ t_2 & 0 & l_2 & 0 & \cdots \\ t_3 & 0 & 0 & l_3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \to \cdots$$

and so

$$\left|G_O^{(n)}\right| = \left(t_t - \frac{t_1^2}{l_1} - \cdots - \frac{t_{n-1}^2}{l_{n-1}}\right) \prod_{k=1}^{n-1} l_k.$$

Computing

$$\lim_{n\to\infty}\sqrt{\frac{\left|G_F^{(n)}\right|}{\left|G_O^{(n)}\right|}}$$

can be done by using some well-known identities for infinite sums and products, and are omitted here. The result is $P_{rf}=(1/\sqrt{\cosh(\omega T)})$. Combining this with the result for V_T and the fact that $\psi(T)$ equals $(P_{rf}/\sqrt{2\pi V_T})\exp(-(x^2/2V_T))$ yields the well-known imaginary time harmonic oscillator propagator

$$U(x,T;0,0)=\sqrt{\frac{m\omega}{2\pi\sinh(\omega T)}}\exp\left(-\frac{m\omega\cosh(\omega T)}{2\sinh(\omega T)}x^2\right).$$

The propagator for the case in which the initial condition is not $x=0$ can be handled similarly – see Appendix I.

3.3 *What is the uncertainty of a quantum particle's velocity?*

Just as the uncertainty for the particle's location at time T can be computed from the norm squared of the functional assigning to each path $x(t)$ the value at its endpoint $x(T)$, one may try and compute the uncertainty of the particle's velocity at time T, which is given by the norm squared of the functional $x(t)\to x'(T)$. However, proceeding as in equations (5 to 5‴) yields a series which does not converge and hence the functional does not have a reproducing kernel in the space of allowed paths. Alternatively, the norm squared of the functional equals

$$\sup_{x(t)}\frac{x'(T)^2}{\|x\|^2}=\left(\frac{2}{m}\right)\sup_{x(t)}\frac{x'(T)^2}{\int_0^T\left[x'(t)^2+\omega^2x^2(t)\right]\mathrm{d}t}$$

and this can be seen to be infinite: for every $\varepsilon>0$, define the path

$$x_\varepsilon(t)=\left\{\begin{array}{l}0\le t\le T-\varepsilon\\(x-T+\varepsilon)^2T-\varepsilon\le t\le T\end{array}\right\}$$

note that $x_\varepsilon(t)$ is differentiable since the derivatives from left and right at $T-\varepsilon$ are both zero. It is straightforward to see that

$$\left(\frac{2}{m}\right)\frac{x_\varepsilon'(T)^2}{\int_0^T\left[x_\varepsilon'(t)^2+\omega^2x_\varepsilon^2(t)\right]\mathrm{d}t}=\frac{120}{\varepsilon m(20\omega^2+3\varepsilon^2)},$$

which tends to infinity as ε tends to zero. Hence the supremum is infinite, and therefore the uncertainty in the particle's velocity is infinite. This is not really a new result (e.g. [1]) but the reproducing kernel formalism allows to derive it in a very natural fashion.

4. Finite-dimensional approximation: the time-dependent oscillator

It is well-known that the propagator can be computed explicitly only in a very small number of cases. Therefore, there is a considerable interest in efficient approximation methods, such as Monte-Carlo integration. Another direction is to search for a finite-dimensional subspace such that the integral over it approximates the integral over the entire space. Some representative research in both directions is presented in [6–13]. The rest of this section discusses a natural family of Fourier subspaces for approximating the propagator of the time-dependent harmonic oscillator, which has drawn considerable interest. It is known that the Schrödinger equation can be solved in this case by introducing further differential equations, but these cannot always be solved explicitly (see [14] which also contains a survey of other works).

A bound on the approximation accuracy is provided. The intuitive idea is that, if the potential is smooth enough, the high frequencies of the paths do not play a significant role.

For the time-dependent oscillator, the inner product corresponding to the action is given by $(x, y)_O = (m/2)\int_0^T [x'(t)y'(t) + \omega(t)x(t)y(t)]\mathrm{d}t$ and it is, in general, impossible to calculate exactly the reproducing kernel and the quantities P_{rf} and V_T, for the following reason. While the Grammian $G_O^{(n)}$ was 'nearly diagonal' for a suitable choice of basis in the time-independent case, that is not so in the time-dependent case. This makes the computation of the reproducing kernel, as well as $|G_O^{(n)}|$, more difficult. However, under some assumptions, it is possible to obtain reasonable finite-dimensional approximations to the two quantities which determine the wave function – V_T and P_{rf}. The bases for these sub-spaces are the same as that used in section 3. Intuitively, these bases are 'nearly orthogonal' under the inner product used, which accounts for the quick convergence as the subspace dimension increases.

4.1 *Assumption on the potential*

It is henceforth assumed that the time-dependent part of the oscillator potential (i.e., the frequency) varies slowly enough in time so that its Fourier coefficients decrease as a power of the Fourier coefficient. Formally, assume that there exist constants $C_1 > 0,\ d > 0$ such that for every $T > 0$ and every integer l,

$$\left|\int_0^T \omega(t)\sin\left(\frac{l\pi t}{T}\right)\mathrm{d}t\right|, \quad \left|\int_0^T \omega(t)\cos\left(\frac{l\pi t}{T}\right)\mathrm{d}t\right| \le \frac{C_1 T}{l^d} \tag{7}$$

$$\left|\int_0^T t\omega(t)\sin\left(\frac{l\pi t}{T}\right)\mathrm{d}t\right|, \quad \left|\int_0^T t\omega(t)\cos\left(\frac{l\pi t}{T}\right)\mathrm{d}t\right| \le \frac{C_1 T^2}{l^d} \tag{7'}$$

the extra T in equation (7′) is due to the extra t in the integrand.

Since

$$\sin\left(\frac{l\pi t}{T}\right)\sin\left(\frac{k\pi t}{T}\right) = \frac{\cos((l-k)\pi t)/T - \cos((l+k)\pi t)/T}{2},$$

it immediately follows that if $k > l > 0$, then

$$\left| \int_0^T \omega(t) \sin\left(\frac{l\pi t}{T}\right) \sin\left(\frac{k\pi t}{T}\right) \mathrm{d}t \right| \leq \frac{1}{2}\left(\frac{C_1 T}{(k-l)^d} + \frac{C_1 T}{(k+l)^d}\right) \leq \frac{C_1 T}{(k-l)^d} \qquad (7'')$$

4.2 *Subspaces used for approximation*

The set of increasing subspaces used for approximating the propagator uses the basis introduced in section 3:

$$V_n = \mathrm{span}\left\{ t, \sin\left(\frac{\pi t}{T}\right), \sin\left(\frac{2\pi t}{T}\right), \ldots, \sin\left(\frac{\pi(n-1)t}{T}\right) \right\}$$

(see also [6]). The rest of this section is devoted to proving that the quantities V_T and P_{rf} can be approximated by computing them on V_n. It is shown that these quantities, when computed on V_n, differ from the values on the entire function space by a factor no greater than $1 + (1/n^{1+\min\{2,2d\}})$.

4.2.1 Approximating V_T. First, a few definitions:

- For the sake of brevity, let us drop the O subscript from the oscillator inner product, so unless specified otherwise it will be denoted hereafter by $(x, y) = (m/2)\int_0^T [x'(t)y'(t) + \omega(t)x(t)y(t)]\mathrm{d}t$ (the $(m/2)$ factor will be left out since it does not affect the results of this section). Denote $(x, y)_F = \int_0^T x'(t)y'(t)\mathrm{d}t$. Note that since $\omega(t) \geq 0$, $\|x\|^2 \geq \|x\|_F^2$ for every $x(t)$.
- Denote by K_n the reproducing kernel for the evaluation at T under the inner product (x, y), restricted to V_n. This means that K_n is the (only) function in V_n which satisfies $(K_n, x) = x(T)$ for every function (path) $x(t) \in V_n$.
- If K_{n+1} denotes the reproducing kernel for V_{n+1}, define the 'residual' $\Delta_n \equiv K_{n+1} - K_n$.
- For brevity, denote $s_{n+1} \equiv \sin(n\pi t/T)$. Note that $V_{n+1} = \mathrm{span}\{V_n, s_{n+1}\}$.

A few lemmas follow. Before proceeding with the technicalities, some motivation. The idea is to prove that Δ_n, the 'residual' between the reproducing kernels for V_n and V_{n+1}, is nearly parallel to s_{n+1}. This follows from the fact that s_{n+1}, which is the 'residual' between V_n and V_{n+1}, is nearly perpendicular to V_n. It is well-known that an orthogonal basis allows to obtain good approximations to the norm squared of a functional; if the orthogonal basis is $\{u_l\}$, the norm squared of the functional F is $\sum_{l=1}^{\infty}(F^2(u_l)/\|u_l\|^2)$, and usually the summands decrease quickly enough so that truncating the infinite sum quickly allows a good approximation. So, one could consider using a Gram–Schmidt process to construct an orthogonal basis; but alas, it will have to be recomputed for every T. Here, the basis is 'almost orthogonal' (Lemma 4), which allows to obtain good finite-dimensional approximations.

LEMMA 1 $\Delta_n \in V_n^{\perp}$.

Proof Let $v_n \in V_n$. Then $(K_n, v_n) = v_n(T)$. Since $v_n \in V_{n+1}$ also, then $(K_{n+1}, v_n) = v_n(T)$. But $(K_{n+1}, v_n) = (K_n + \Delta_n, v_n) = (K_n, v_n) + (\Delta_n, v_n) = v_n(T) + (\Delta_n, v_n)$, so $(\Delta_n, v_n) = 0$.

LEMMA 2 $\|s_{n+1}\|^2 \geq (\pi^2 n^2/2T)$.

Proof

$$\|s_{n+1}\|^2 \geq \|s_{n+1}\|_F^2 = \int_0^T \left[\sin\left(\frac{n\pi t}{T}\right)'\right]^2 \mathrm{d}t = \frac{\pi^2 n^2}{2T}.$$

LEMMA 3 *Let* $v_n \in V_n$, *denote* $v_n = a_0 t + \sum_{l=1}^{n-1} a_l \sin(\pi l t/T)$. *Then* $\|v_n\|^2 \geq a_0^2 T + (\pi^2/2T)\sum_{l=1}^{n-1} l^2 a_l^2$.

Proof $\|v_n\|^2 \geq \|v_n\|_F^2$, but all the summands of v_n are orthogonal under $(,)_F$, so $\|v_n\|^2 \geq a_0^2\|t\|_F^2 + \sum_{l=1}^{n-1} a_l^2 \|\sin(l\pi t/T)\|_F^2 = a_0^2 T + (\pi^2/2T)\sum_{l=1}^{n-1} l^2 a_l^2$.

LEMMA 4 *There exists a constant* C_2 *such that if* $v_n \in V_n$, *then*

$$(s_{n+1}, v_n)^2 \leq C_2 \frac{\|v_n\|^2 \|s_{n+1}\|^2}{n^{2+\min\{2d,2\}}} T^4.$$

Proof Denote

$$v_n = a_0 t + a_1 \sin\left(\frac{\pi t}{T}\right) + a_2 \sin\left(\frac{2\pi t}{T}\right) + \cdots + a_{n-1} \sin\left(\frac{(n-1)\pi t}{T}\right).$$

Since

$$(t, s_{n+1})_F = \left(\sin\left(\frac{\pi t}{T}\right), s_{n+1}\right)_F = \cdots = \left(\sin\left(\frac{(n-1)\pi t}{T}\right), s_{n+1}\right)_F = 0,$$

the assumptions in equations (7 to 7″) can be used to bound (s_{n+1}, v_n):

$$|(s_{n+1}, v_n)| \leq |a_0(t, s_{n+1})| + \sum_{l=1}^{n-1} \left|a_l\left(\sin\left(\frac{l\pi t}{T}\right), s_{n+1}\right)\right| \leq C_1\left[\frac{|a_0|T^2}{n^d} + \sum_{l=1}^{n-1}\frac{|a_l|T}{(n-l)^d}\right].$$

Since for every $A, B \geq 0$, $(A+B)^2 \leq 2(A^2+B^2)$, then

$$(s_{n+1}, v_n)^2 \leq 2C_1^2\left[\frac{a_0^2 T^4}{n^{2d}} + \left(\sum_{l=1}^{n-1}\frac{|a_l|T}{(n-l)^d}\right)^2\right].$$

Using the Cauchy–Schwartz inequality,

$$\left(\sum_{l=1}^{n-1}\frac{|a_l|T}{(n-l)^d}\right)^2 = T^2\left(\sum_{l=1}^{n-1} l|a_l|\frac{1}{l(n-l)^d}\right)^2 \leq T^2\left(\sum_{l=1}^{n-1} l^2 a_l^2\right)\left(\sum_{l=1}^{n-1}\frac{1}{l^2(n-l)^{2d}}\right).$$

From Lemma 3, the second product term is bounded by $(2T/\pi^2)\|v_n\|^2$, and it can be shown that the third product term behaves like $1/(n^{\min\{2,2d\}})$ (up to a constant which varies very slowly as a function of d). Since $\|s_{n+1}\|^2 \geq (\pi^2 n^2/2T)$ (Lemma 2), it follows that $(\sum_{l=1}^{n-1}((|a_l|T)/(n-l)^d)^2$ is bounded from above by a constant times

$T^4/(n^{2+\min\{2,2d\}})\|s_{n+1}\|^2\|v_n\|^2$. $2C_1^2[a_0^2T^4/n^{2d}]$, the other summand compromising the bound for $(s_{n+1}, v_n)^2$, can be bounded by observing that $\|v_n\|^2 \geq a_0^2 T$ (Lemma 3) and $\|s_{n+1}\|^2 \geq (\pi^2 n^2/2T)$ (Lemma 2), hence

$$2C_1^2\left[\frac{a_0^2T^4}{n^{2d}}\right] = \frac{2C_1^2T^4\left(a_0^2T\right)\left(\pi^2n^2/T\right)}{\pi^2n^2n^{2d}} \leq \frac{2C_1^2}{\pi^2n^{2+2d}}\|v_n\|^2\|s_{n+1}\|^2$$

which concludes the proof. For brevity, denote the bound (with the T powers in the numerator and the power of n in the denominator thrown in) by $C(n)$. To summarize then, if $v_n \in V_n$, then $(s_{n+1}, v_n)^2 \leq C(n)\|v_n\|^2\|s_{n+1}\|^2$. Since for large n, $C(n)$ is very small, v_n and s_{n+1} are indeed 'nearly orthogonal', since their inner product is far smaller than the product of their norms.

LEMMA 5 $(\Delta_n, s_{n+1})^2 \geq [1 - C(n)]\|\Delta_n\|^2\|s_{n+1}\|^2$.

Proof Since $V_{n+1} = V_n \oplus \text{span}\{\Delta_n\}$ (Lemma 1), s_{n+1} can be (uniquely) represented as $s_{n+1}^{V_n} + s_{n+1}^{\Delta_n}$, with $s_{n+1}^{V_n} \in V_n$, $s_{n+1}^{\Delta_n} \in \text{span}\{\Delta_n\}$. It is well-known from linear algebra that $\|s_{n+1}\|^2 = \|s_{n+1}^{V_n}\|^2 + \|s_{n+1}^{\Delta_n}\|^2$, and that

$$\left\|s_{n+1}^{V_n}\right\|^2 = \frac{\left(s_{n+1}, s_{n+1}^{V_n}\right)^2}{\left\|s_{n+1}^{V_n}\right\|^2}.$$

But from Lemma 4,

$$\frac{\left(s_{n+1}, s_{n+1}^{V_n}\right)^2}{\left\|s_{n+1}^{V_n}\right\|^2} \leq C(n)\|s_{n+1}\|^2,$$

from which the proof follows immediately.

LEMMA 6 $(K_n, s_{n+1})^2 = (\Delta_n, s_{n+1})^2$.

Proof Since $s_{n+1}(T) = 0$, $(K_{n+1}, s_{n+1}) = 0$. But $(K_{n+1}, s_{n+1}) = (K_n, s_{n+1}) + (\Delta_n, s_{n+1})$, hence $(K_n, s_{n+1}) = -(\Delta_n, s_{n+1})$, and squaring both sides concludes the proof.

LEMMA 7 $C(n)/(1 - C(n))\|K_n\|^2 \geq \|\Delta_n\|^2$.

Proof Using the fact that $K_n \in V_n$ and Lemma 4, $(K_n, s_{n+1})^2 \leq C(n)\|K_n\|^2\|s_{n+1}\|^2$. Combining this with Lemmas 5 and 6 yields

$$C(n)\|K_n\|^2\|s_{n+1}\|^2 \geq (K_n, s_{n+1})^2 \underset{\text{Lemma 6}}{=} (\Delta_n, s_{n+1})^2 \underset{\text{Lemma 5}}{\geq} (1 - C(n))\|\Delta_n\|^2\|s_{n+1}\|^2,$$

from which the proof follows by cancelling out $\|s_{n+1}\|^2$ and dividing by $1 - C(n)$.

Finally, the norm on V_{n+1} can be bounded by the norm on V_n:

THEOREM 1

$$\|K_{n+1}\|^2 \leq \frac{1}{1 - C(n)}\|K_n\|^2.$$

Proof By definition, $K_{n+1} = K_n + \Delta_n$. From Lemma 1, $(K_n, \Delta_n) = 0$, hence

$$\left\|K_{n+1}\right\|^2 = \|K_n\|^2 + \|\Delta_n\|^2 \underset{\text{Lemma 7}}{\leq} \|K_n\|^2\left(1 + \frac{C(n)}{1 - C(n)}\right) = \frac{\|K_n\|^2}{1 - C(n)}.$$

If $C(n) \ll 1$ (which will hold for a large enough n, since $C(n)$ falls rapidly as a function of n), it can be assumed that $\|K_{n+1}\|^2 \leq [1 + C(n)]\|K_n\|^2$.

THEOREM 2 *The norm squared of e_T restricted to V_n approximates the norm squared on the entire Sobolev space to a factor of $1 + C(T^4/n^{1+\min\{2,2d\}})$, where C is a constant.*

Proof In order to bound the ratio between the norm squared restricted to V_n and the norm squared on the entire space, it suffices to multiply the bounds on the ratios between the norm squared restricted to V_N and V_{N+1}, for $n \leq N < \infty$. Using Theorem 1 and bearing in mind that $C(N) \leq (CT^4/N^{2+\min\{2,2d\}})$ for some constant C, the infinite product over this range of N is bounded by (use $\exp(\alpha) \approx (1 + \alpha)$ for $\alpha \ll 1$)

$$\begin{aligned}\prod_{N=n}^{\infty}\left(1 + C\frac{T^4}{N^{2+\min\{2,2d\}}}\right) &\cong \prod_{N=n}^{\infty}\exp\left(C\frac{T^4}{N^{2+\min\{2,2d\}}}\right)\\ &= \exp\left(\sum_{N=n}^{\infty} C\frac{T^4}{N^{2+\min\{2,2d\}}}\right)\\ &\cong \exp\left(C\frac{T^4}{n^{1+\min\{2,2d\}}}\right) \cong 1 + C\frac{T^4}{n^{1+\min\{2,2d\}}}.\end{aligned}$$

Note that if $d \geq 1$, the approximation error is of the order $1/n^3$, which is the same order of approximation obtained for the simple harmonic oscillator (see section 3).

Note that the bound increases with T – this is because as T increases, more and more paths are allowed to 'enter the game'; there will be more paths with a small action (i.e., small derivatives) and with greater variance at the endpoint, and thus a higher-dimensional subspace is required to obtain a good approximation. As is shown next, under reasonable assumptions, the T^4 factor is not of great concern when approximating P_{rf}, since P_{rf} decreases much more rapidly. Also, other conditions than those assumed in equations (7 and 7′) may yield bounds which depend on a lower power of T.

4.2.2 Approximating P_{rf}. In section 3 (equation (6)) it was shown that the 'probability reduction factor' equals

$$P_{rf} = \lim_{n\to\infty}\sqrt{\frac{\left|G_F^{(n)}\right|}{\left|G^{(n)}\right|}},$$

where $G^{(n)}$ and $G_F^{(n)}$ are, respectively, the Grammians of the oscillator and free particle inner product:

$$\left|G_{k,l}^{(n)}\right| = (\beta_k, \beta_l) \quad \text{and} \quad \left|G_{F_{k,l}}^{(n)}\right| = (\beta_k, \beta_l)_F.$$

It was also shown that

$$\left|G_F^{(n)}\right| = T\prod_{k=1}^{n-1}\frac{\pi^2 k^2}{2T}$$

(here $m = 1$). In order to estimate the quality of approximation of P_{rf} on V_n, one can first study the ratio between the approximations on V_{n+1} and V_n, which equals

$$\left(\frac{\left|G_F^{(n+1)}\right|}{\left|G^{(n+1)}\right|}\Big/\frac{\left|G_F^{(n)}\right|}{\left|G^{(n)}\right|}\right)^{1/2} = \left(\frac{\left|G_F^{(n+1)}\right|}{\left|G^{(n+1)}\right|}\frac{\left|G^{(n)}\right|}{\left|G_F^{(n)}\right|}\right)^{1/2} = \left(\frac{\pi^2 n^2}{2T}\frac{\left|G^{(n)}\right|}{\left|G^{(n+1)}\right|}\right)^{1/2} \tag{8}$$

The next step is to bound $|G^{(n+1)}|$ from both sides. Had the basis

$$\left\{\beta_0 = t, \beta_1 = \sin\left(\frac{\pi t}{T}\right), \beta_2 = \sin\left(\frac{2\pi t}{T}\right), \ldots\right\}$$

been orthogonal, the task would be simple, as then $|G^{(n+1)}| = \|\beta_n\|^2|G^{(n)}|$ would hold. But although the basis is not orthogonal, it is 'nearly orthogonal', since – as proved in Lemma 4 – the norm squared of the projection of $s_{n+1} = \beta_n$ on V_n is bounded from above by

$$C_2\frac{T^4}{n^{2+\min\{2d,2\}}}\|s_{n+1}\|^2.$$

This can be used via the following.

LEMMA 8 *Denote the projection of β_n on V_n by $\beta_n^{V_n}$ (so for every $0 \le l \le n-1$, $(\beta_n - \beta_n^{V_n}, \beta_l) = 0$). Then $|G^{(n+1)}| = (\beta_n, \beta_n - \beta_n^{V_n})|G^{(n)}|$.*

Proof Let $\beta_n^{V_n} = \sum_{k=0}^{n-1} a_k\beta_k$. Denote the rows of $G^{(n+1)}$ by $\{L_0, L_1, \ldots, L_n\}$. The determinant is preserved under $L_n \to L_n - \sum_{k=0}^{n-1} a_k L_k$, which changes the lth element of the last row thusly:

$$\begin{aligned}(\beta_l, \beta_n) \to (\beta_l, \beta_n) - \sum_{k=0}^{n-1} a_k(\beta_l, \beta_k) &= \left(\beta_l, \beta_n - \sum_{k=0}^{n-1} a_k\beta_k\right)\\ &= \left(\beta_l, \beta_n - \beta_n^{V_n}\right) = \begin{cases} 0 & l < n\\ (\beta_n, \beta_n - \beta_n^{V_n}) & l = n\end{cases}\end{aligned}$$

and the proof follows immediately by expanding the determinant by the last row.

From Lemma 4, it follows that $[1 - C(n)]\|\beta_n\|^2 \le (\beta_n, \beta_n - \beta_n^{V_n}) \le \|\beta_n\|^2$.

From equation (8), and since $\beta_n = s_{n+1}$, it follows that

$$[1 - C(n)]\frac{\pi^2 n^2}{2T\|s_{n+1}\|^2} \le \frac{\left|G_F^{(n+1)}\right|}{\left|G^{(n+1)}\right|}\Big/\frac{\left|G_F^{(n)}\right|}{\left|G^{(n)}\right|} \le \frac{\pi^2 n^2}{2T\|s_{n+1}\|^2} \tag{9}$$

Now,

$$\|s_{n+1}\|^2 = \int_0^T\left[\sin'\left(\frac{n\pi t}{T}\right)^2 + \omega(t)\sin^2(n\pi t)\right]\mathrm{d}t = \frac{\pi^2 n^2}{2T} + \int_0^T\left[\omega(t)\left(\frac{1-\cos(2n\pi t)}{2}\right)\right]\mathrm{d}t.$$

Denoting $\int_0^T \omega(t)\mathrm{d}t \equiv W(T)$ and using equation (7) yields

$$\frac{\pi^2 n^2}{2T} + \frac{W(T)}{2} - \frac{C_1 T}{n^d} \leq \|s_{n+1}\|^2 \leq \frac{\pi^2 n^2}{2T} + \frac{W(T)}{2} + \frac{C_1 T}{n^d}$$

$$\Rightarrow \frac{1}{1 + (TW(T)/\pi^2 n^2) + (2C_1 T^2/\pi^2 n^{d+2})} \leq \frac{\pi^2 n^2}{2T\|s_{n+1}\|^2}$$

$$\leq \frac{1}{1 + (TW(T)/\pi^2 n^2) - (2C_1 T^2/\pi^2 n^{d+2})}$$

and if n is large enough, use $1/(1+\alpha) \approx 1 - \alpha$ for $\alpha \ll 1$ to obtain

$$1 - \frac{TW(T)}{\pi^2 n^2} - \frac{2C_1 T^2}{\pi^2 n^{d+2}} \leq \frac{\pi^2 n^2}{2T\|s_{n+1}\|^2} \leq 1 - \frac{TW(T)}{\pi^2 n^2} + \frac{2C_1 T^2}{\pi^2 n^{d+2}}.$$

Combining this with equation (9) yields

$$[1 - C(N)]\left(1 - \frac{TW(T)}{\pi^2 N^2} - \frac{2C_1 T^2}{\pi^2 N^{d+2}}\right) \leq \frac{\left|G_F^{(N+1)}\right|}{\left|G^{(N+1)}\right|} \Bigg/ \frac{\left|G_F^{(N)}\right|}{\left|G^{(N)}\right|} \leq 1 - \frac{TW(T)}{\pi^2 N^2} + \frac{2C_1 T^2}{\pi^2 N^{d+2}} \tag{10}$$

As before, in order to estimate the value of the approximation on V_n, one has to estimate the infinite product of the upper and lower bounds in equation (10), for $n \leq N < \infty$. Proceeding as before, the bound for the $1 - C(N)$ factor is $1 - C(T^4/n^{1+\min\{2,2d\}})$ for some constant C. It remains to bound

$$\prod_{N=n}^{\infty}\left(1 - \frac{TW(T)}{\pi^2 N^2} - \frac{2C_1 T^2}{\pi^2 N^{d+2}}\right)$$

and

$$\prod_{N=n}^{\infty}\left(1 - \frac{TW(T)}{\pi^2 N^2} + \frac{2C_1 T^2}{\pi^2 N^{d+2}}\right).$$

However, these expressions have no unknown factors such as $C(N)$; in some cases (e.g. $d = 2$) they can be computed explicitly, or they can be estimated using the approximation

$$1 - \frac{TW(T)}{\pi^2 N^2} + \frac{2C_1 T^2}{\pi^2 N^{d+2}} \approx \left(1 - \frac{TW(T)}{\pi^2 N^2}\right)\left(1 + \frac{2C_1 T^2}{\pi^2 N^{d+2}}\right).$$

It follows then that P_{rf} can be approximated with the same accuracy as V_T.

Remark If one is interested in the ground state energy, the T^4 factor is usually of no concern, since P_{rf} is much smaller than $(1/T^4)$. For example, if $\omega(t)$ is bounded from below by a constant $K > 0$, then the norm squared of the corresponding inner product is bounded from below by the norm squared of the corresponding simple oscillator norm with $\omega = \sqrt{K}$; since larger norm means

smaller probability reduction factor (equation (3)), the probability reduction factor for the time-dependent oscillator is bounded from above by the probability reduction factor for the simple oscillator with $\omega = \sqrt{K}$, which equals $(1/\cosh(\sqrt{K}T))$, hence a good approximation can be obtained in a low-dimensional subspace.

5. Concluding remarks and future work

A reproducing kernel approach was applied to calculate the free particle and simple harmonic oscillator propagators. It was shown that the propagator at any time T is a Gaussian; as such, it is determined by its variance and a multiplicative factor. The variance is half the value of the reproducing kernel at $t = T$, and the multiplicative factor (probability reduction factor) equals

$$\frac{\int_{x(t)} \exp(-S[x(t)])Dx(t)}{\int_{x(t)} \exp(-S_F[x(t)])Dx(t)},$$

where $S[x(t)]$ resp. $S_F[x(t)]$ are the actions of the harmonic oscillator resp. free particle.

In this case, the reproducing kernel and 'probability reduction factor' can be calculated exactly. For the time-dependent oscillator, such a calculation is impossible, in general. However, if the oscillator frequency changes slowly enough in time, then an efficient finite-dimensional approximation can be constructed, using the fact that the variance is half the norm squared of the evaluation functional at T. An increasing sequence of finite-dimensional subspaces is chosen so that the 'increment' between successive subspaces has a relatively small value at T, but a large norm; this allows to bound the ratio between the functional's norm on successive subspace, and by multiplying these bounds, the ratio between the norm on subspaces and the entire space can also be bounded. This also allows to approximate the ground state energy.

It was also shown that the functional assigning to each path its derivative at T is unbounded, which proves that the uncertainty associated with the particle's velocity is infinite.

Some possibilities for future research are:

- Can the finite-dimensional approximations be improved? It is possible that there are better bases than the Fourier one, for some potentials. Also, it may be the case that the asymptotic behaviour of the Fourier (or other) coefficients of the potentials is known (and not only an upper bound). That will allow to better approximate the variance and 'probability reduction factor'.
- Non-quadratic potentials. Although the Gaussian integral formalism does not apply in this case, it may be possible to derive good finite-dimensional approximations using the same idea employed here – seek an increasing sequence of subspaces such that the 'increments' have a large action and a small value for the evaluation functional.
- Treat variation in time of the oscillator frequency which is not smooth (e.g. step function, a sum of delta functions).

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Appendix I: $U(x, T; x_0, 0)$ for $x_0 \neq 0$

So far, it was assumed that $\psi(0) = \delta(x)$, which meant that the integration was performed over the space of paths $x(t)$ satisfying $x(0) = 0$. In order to find the general propagator, assume $x(0) = x_0$. The computation proceeds very much like before; alas, care should be taken; because now the space of paths is obviously not a linear space, and the results on integration over Hilbert spaces cannot be used directly. In order to compute the integral, a change of variable is performed which maps the space to the space of paths satisfying $x(0) = 0$, while preserving the probability associated with the paths satisfying $x(0) = x_0$. The details follow.

Define $P_{x_0} = \{x(t)|\ x(0) = x_0\},\ P_0 = \{x(t)|\ x(0) = 0\}$. In order to compute the expectation at T, one needs to compute $\int_{P_{x_0}} x(T) \exp(-\|x\|^2) Dx$, under the normalization $\int_{P_{x_0}} \exp(-\|x\|^2) Dx = 1$. Denote by h_{x_0} the path satisfying $x(t) = x_0$ for all t. Under the translation $x(t) \to x(t) - h_{x_0}$, the integral transforms to $\int_{P_0} [x(T) + x_0] \times \exp(-\|x + h_{x_0}\|^2) Dx$ under the normalization $\int_{P_0} \exp(-\|x + h_{x_0}\|^2) Dx = 1$, or simply

$$\frac{\int_{P_0} [x(T) + x_0] \exp\left(-\|x + h_{x_0}\|^2\right) Dx}{\int_{P_0} \exp\left(-\|x + h_{x_0}\|^2\right) Dx} = x_0 + \frac{\int_{P_0} x(T) \exp\left(-\|x + h_{x_0}\|^2\right) Dx}{\int_{P_0} \exp\left(-\|x + h_{x_0}\|^2\right) Dx}$$
$$= x_0 + \frac{\int_{P_0} (x, e_T) \exp\left(-\|x + h_{x_0}\|^2\right) Dx}{\int_{P_0} \exp\left(-\|x + h_{x_0}\|^2\right) Dx}$$

according to the theory of Gaussian integrals and cylindrical measures [10], the integral can be reduced to a one-dimensional integral over span$\{e_T\}$, and it equals $-(h_{x_0}, e_T)$ (note that this does not equal $-h_{x_0}(T)$, since e_T is the reproducing kernel for P_0, not P_{x_0}). According to the definition of the inner product in P_0 (equation (2)), $(h_{x_0}, e_T) = (m\omega^2 x_0/2)\int_0^T e_T(t)\mathrm{d}t$. This integral can be computed using standard results on infinite sums, and the expectation turns out to be $(x_0/\cosh(\omega T))$. Similarly V_T and P_{rf} can be computed.

Appendix II: Computing the ground state energy

The imaginary time propagator is given by $U(T;0) = \sum_{n=0}^{\infty} \exp(-E_n t)|E_n\rangle\langle E_n|$, where E_n is the nth energy level and $|E_n\rangle$ resp. $\langle E_n|$ the ket resp. bra nth energy eigenstate.

So, for large T, $U(T;0) \approx \exp(-E_0 T)|E_0\rangle\langle E_0|$. If the initial state is the delta function, then the state at T is $U(T;0)\big|\delta(x)\big\rangle \approx (\exp(-E_0 T)|E_0\rangle\langle E_0|)\big|\delta(x)\big\rangle = \exp(-E_0 T)E_0(0)|E_0\rangle$, where $(|E_0\rangle)(0)$ is replaced by the more convenient notation $E_0(0)$. Using the results of section 2,

$$\exp(-E_0 T)E_0(0)|E_0\rangle \approx \frac{P_{rf}}{\sqrt{2\pi V_T}}\exp\left(-\frac{x^2}{2V_T}\right).$$

Assuming $|E_0\rangle$ is normalized, then since $|E_0\rangle$ roughly equals $\exp(-(x^2/2V_T))$ up to a scale factor, it follows immediately that $|E_0\rangle \approx (\pi V_T)^{-(1/4)}\exp(-(x^2/2V_T))$, and therefore $\exp(-E_0 T)E_0(0)|E_0\rangle \approx \exp(-E_0 T)(\pi V_T)^{-(1/2)}\exp(-(x^2/2V_T))$, hence $\exp(-E_0 T) \approx (P_{rf}/\sqrt{2}) \Rightarrow E_0 \approx -(\log(P_{rf})/T)$ for large enough T. Thus, the ground state energy can be approximated to within a desired accuracy using the results derived in section 4 for the approximation of P_{rf}.