The study of the dynamics of quantum bipartite entangled systems using Feynman path integrals

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The generalized Gaussian integrals

1.1 Preliminary form

A Gaussian integral is the integral of the Gaussian function $\exp[-x^2]$:

$$\int_{\infty}^{-\infty} \exp[-x^2]\, \mathrm{d}x = \sqrt{\pi}. \tag{1.1}$$

However, this is not that useful for path integrals, because it demands a more generalized form of this Gaussian function. Therefore, we focus on integrals of the form

$$I_1 = \int_{\infty}^{-\infty} x^n \exp[-(ax^2 + bx + c)]\, \mathrm{d}x\,, \tag{1.2}$$

where a, b, and c are constants and n is a positive integer. This integral will be very useful later on when evaluating the Born expansion of the propagator.

Because we're just going to be dealing with integrals from negative to positive infinity, I shall omit the bounds of the integrals. Thus, every integral written with no bounds from now on are assumed to be a definite integral from negative to positive infinity.

1.2 Evaluation

To evaluate I_1 (eq. (1.2)), we shall complete the square first, then substitute the exponents to fit the form of the standard Gaussian integral.

$$\int x^n \mathrm{e}^{-(ax^2+bx+c)}\, \mathrm{d}x = \int x^n \exp\left[-a\left(x + \frac{b^2}{2a}\right)^2 + \frac{b^2}{4a} - c\right] \mathrm{d}x$$

$$= \mathrm{e}^{\frac{b^2}{4a}-c} \int x^n \exp\left[-a\left(x + \frac{b^2}{2a}\right)\right] \mathrm{d}x\,.$$

Let

$$-u^2 = -a\left(x + \frac{b^2}{2a}\right)^2 \tag{1.3}$$

$$x = \frac{u}{\sqrt{a}} - \frac{b^2}{2a} \tag{1.4}$$

$$\frac{\mathrm{d}x}{\mathrm{d}u} = \frac{\mathrm{d}}{\mathrm{d}u}\left(\frac{u}{\sqrt{a}} - \frac{b^2}{2a}\right) \tag{1.5}$$

$$\mathrm{d}x = \frac{1}{\sqrt{a}}\,\mathrm{d}u\,. \tag{1.6}$$

Then,

$$I_1 = \mathrm{e}^{\frac{b^2}{4a}-c}\frac{1}{\sqrt{a}}\int\left(\frac{u}{\sqrt{a}} - \frac{b^2}{2a}\right)^n \mathrm{e}^{-u^2}\,\mathrm{d}u\,. \tag{1.7}$$

$$= \mathrm{e}^{\frac{b^2}{4a}-c}\frac{1}{\sqrt{a}}\int\sum_{k=0}^{n}\binom{n}{k}\left(\frac{b^2}{2a}\right)^{n-k}\left(\frac{u}{\sqrt{a}}\right)^k \mathrm{e}^{-u^2}\,\mathrm{d}u\,. \tag{1.8}$$

$$= \mathrm{e}^{\frac{b^2}{4a}-c}\frac{1}{\sqrt{a}}\sum_{k=0}^{n}\left[\binom{n}{k}\left(\frac{b^2}{2a}\right)^{n-k}\left(\frac{1}{\sqrt{a}}\right)^k\int u^k \mathrm{e}^{u^2}\,\mathrm{d}u\right], \tag{1.9}$$

i.e., I_1 can be written as a sum of

$$I_0 = \int u^k \mathrm{e}^{-u^2}\,\mathrm{d}u\,. \tag{1.10}$$

Notice that when n is odd, the integrand of I_0 is an odd function. Therefore, I_0 is zero whenever n is odd. When n is even however, the integrand is even. Thus, it can be simplified to

$$2\int_0^\infty u^{2m}\mathrm{e}^{-u^2}\,\mathrm{d}u \tag{1.11}$$

where $k = 2m$. We then do another substitution by letting $-t = -u^2$. Thus, $u = \sqrt{t}$ and $\mathrm{d}u = \mathrm{d}t/2\sqrt{t}$. Both infinity and zero aren't affected by a square root, therefore the bound doesn't change. Our integral then becomes

$$2\times\int_0^\infty t^m \mathrm{e}^{-t}\frac{1}{2\sqrt{t}}\,\mathrm{d}t\,. \tag{1.12}$$

$$= \int_0^\infty t^{m-\frac{1}{2}}\mathrm{e}^{-t}\,\mathrm{d}t \tag{1.13}$$

$$= \int_0^\infty t^{m+\frac{1}{2}-1}\mathrm{e}^{-t}\,\mathrm{d}t \tag{1.14}$$

$$= \Gamma\left(m + \frac{1}{2}\right) \tag{1.15}$$

$$= \Gamma\left(\frac{k+1}{2}\right). \tag{1.16}$$

Since the integral evaluates to the gamma function for only even numbers, we add a term that makes $I_0 = 0$ when n is odd:

$$I_0 = \frac{1}{2}((-1)^k + 1)\,\Gamma\left(\frac{k+1}{2}\right). \tag{1.17}$$

Thus, from eq. (1.9),

$$I_1 = \mathrm{e}^{\frac{b^2}{4a}-c}\frac{1}{\sqrt{a}}\sum_{k=0}^{n}\left[\binom{n}{k}\left(\frac{b^2}{2a}\right)^{n-k}\left(\frac{1}{\sqrt{a}}\right)^k\frac{1}{2}((-1)^k + 1)\,\Gamma\left(\frac{k+1}{2}\right)\right] \tag{1.18}$$

To continue this, we then expand the combinatorics and use the formulas of arguments with half-integer real part to get

$$e^{\frac{b^2}{4a}-c}\frac{1}{\sqrt{a}}\sum_{k=0}^{n}\frac{n!}{k!(n-k)!}\left(\frac{b^2}{2a}\right)^n\left(\frac{2a}{b^2}\right)^k\left(\frac{1}{\sqrt{a}}\right)^k\left(\sqrt{\pi}\frac{k!}{4^{\frac{k}{2}}(k/2)!}\right)$$
$$\times\frac{1}{2}((-1)^k+1) \tag{1.19}$$

$$= e^{\frac{b^2}{4a}-c}n!\sqrt{\frac{\pi}{a}}\left(\frac{b^2}{2a}\right)^n\sum_{k=0}^{n}\frac{1}{(n-k)!(k/2)!}\left(\frac{\sqrt{a}}{b^2}\right)^k\frac{1}{2}((-1)^k+1) \tag{1.20}$$

To simplify the summation, we replace k with $2k$, and the upper limit with m where $m = \lfloor n/2 \rfloor$. Thus, we get

$$\left[\sum_{k=0}^{m}\frac{1}{(n-2k)!k!}\left(\frac{\sqrt{a}}{b^2}\right)^{2k}\right]e^{\frac{b^2}{4a}-c}n!\left(\frac{b^2}{2a}\right)^n\sqrt{\frac{\pi}{a}} \tag{1.21}$$

As far as I know, this equation cannot be simplified further.

Comment on the generalized Gaussian integral   Note that the integral in eq. (1.2) can be casted in the form of Meijer's G function for $n \geq 0$:

$$\int x^n \exp\left[-ax^2 - bx - c\right]\mathrm{d}x$$

$$= \frac{e^{-c}}{2\sqrt{\pi}ab}\left[-\frac{2^{n+1}a}{b^n}G_{2,1}^{1,2}\left(\begin{matrix}\frac{1-n}{2}, -\frac{n}{2}\\0\end{matrix}\middle|\frac{4ae^{-2i\pi}}{b^2}\right) + a^{\frac{1-n}{2}}bG_{1,2}^{2,1}\left(\begin{matrix}\frac{1-n}{2}\\0,\frac{1}{2}\end{matrix}\middle|\frac{b^2}{4a}\right)\right] \tag{1.22}$$

However, this form doesn't seem to be very helpful when we try to evaluate the polynomial part of the Gaussian integral because of the nature of the Meijer's G function that's defined with integral of products.

Originally, I was going to evaluate everything using `SymPy`, and not really care about anything else. However, I came to realize that `SymPy` doesn't bother integrating any Gaussian integrals that have complex number components. My own implementation will be written in chapter 3

1.3   Tables of Gaussian integrals with varying orders

$n = 0$: $+\dfrac{1}{1}\sqrt{\dfrac{\pi}{a}}e^{\frac{b^2}{4a}-c}$

$n = 1$: $-\dfrac{b}{2}\sqrt{\dfrac{\pi}{a^3}}e^{\frac{b^2}{4a}-c}$

$n = 2$: $+\dfrac{1}{4}\sqrt{\dfrac{\pi}{a^5}}(2a+b^2)e^{\frac{b^2}{4a}-c}$

$n = 3$: $-\dfrac{b}{8}\sqrt{\dfrac{\pi}{a^7}}(6a+b^2)e^{\frac{b^2}{4a}-c}$

$n = 4$: $+\dfrac{1}{16}\sqrt{\dfrac{\pi}{a^9}}(12a^2+12ab^2+b^4)e^{\frac{b^2}{4a}-c}$

$$n = 5: \quad -\frac{b}{32}\sqrt{\frac{\pi}{a^{11}}}(60a^2 + 20ab^2 + b^2)\mathrm{e}^{\frac{b^2}{4a}-c}$$

$$n = 6: \quad +\frac{1}{64}\sqrt{\frac{\pi}{a^{13}}}(120a^3 + 180a^2b^2 + 30ab^4 + b^6)\mathrm{e}^{\frac{b^2}{4a}-c}$$

$$n = 7: \quad -\frac{b}{128}\sqrt{\frac{\pi}{a^{15}}}(840a^3 + 420a^2b^2 + 42ab^4 + b^6)\mathrm{e}^{\frac{b^2}{4a}-c}$$

$$n = 8: \quad +\frac{1}{256}\sqrt{\frac{\pi}{a^{17}}}(1680a^4 + 3360a^3b^2 + 840a^2b^4 + 56ab^6 + b^8)\mathrm{e}^{\frac{b^2}{4a}-c}$$

$$n = 9: \quad -\frac{b}{512}\sqrt{\frac{\pi}{a^{19}}}(15120a^4 + 10080a^3b^2 + 1512a^2b^4 + 72ab^6 + b^8)\mathrm{e}^{\frac{b^2}{4a}-c}$$

Propagator and joint probability distribution

2.1 General theory for the propagator of two particles

2.1.1 Non-interacting systems

The propagator for a single particle system is used to find the probability distribution $\tilde{P}(x)$ of a state at anytime, i.e., for a state $|\psi(t_0)\rangle$,

$$\tilde{P}(q_F, t_F) = \langle q_F|\psi(t_F)\rangle = \int (q_0, \Delta t)\psi(q_0, t_0)\,\mathrm{d}q_0\,K. \tag{2.1}$$

When taken the modulus squared, $|\tilde{P}(q_F, t_F)|^2$, or just $P(q_F, t_F)$, represents the probability of finding that particle at the point (q_F, t_F) in spacetime.

We shall then extend this idea to describe a two particle system. Let there be a state ket $|\eta(t)\rangle$, which simultaneously represents the state of both particle one and particle two. Assume that at some point in time, $|\eta\rangle$ is separable:

$$|\eta(t_0)\rangle = |\psi(t_0)\rangle \otimes |\phi(t_0)\rangle. \tag{2.2}$$

If the subsystem of $|\eta\rangle$ is non-interacting, the Hamiltonian must be completely separable, which also implies that the time evolution operator $\hat{U}$ is also separable. Consider $\langle q_F, q'_F|\eta(t_F)\rangle$ where the unprimed q belongs to the position in the Hilbert space of particle one, and the primed q's, in Hilbert space of particle two.

$$
\begin{aligned}
\langle q_F, q'_F|\eta(t_F)\rangle &= \langle q_F, q'_F|\left(|\psi_i(t_F)\rangle\,|\phi_i(t_F)\rangle\right) \\
&= \psi_i(q_F, t_F)\phi_i(q'_F, t'_F) \\
&= \iint K_\psi(q_F, t_F; q_0, t_0)K_\phi(q'_F, t'_F; q'_0, t'_0)\left[\psi_i(q_F, t_F)\phi_i(q'_F, t'_F)\right]\mathrm{d}q_0\,\mathrm{d}q'_0.
\end{aligned}
$$

For most systems, K_ψ and K_ϕ is identical because both ψ_i and ϕ_i is affected by the same potential. But for some, K_ψ and K_ϕ might not be identical. E.g., if ψ is in a potential well, but ϕ is a free particle that's infinitely far away. K_ψ must be of the potential well, and K_ϕ must be of the free particle.

It can be seen that $\langle q_F, q_F' | \eta(t_F) \rangle$ represents the probability distribution of both the two particles. E.g., for a state ket $|\psi\rangle \otimes |\phi\rangle$,

$$(\langle q_F | \ \langle q_F' |)(\ |\psi(t_F)\rangle \ |\phi(t_F')\rangle) \tag{2.3}$$

$$= \langle q_F|\psi(t_F)\rangle \ \langle q_F'|\phi(t_F')\rangle \tag{2.4}$$

$$= \iint \mathrm{d}q_0 \, \mathrm{d}q_0' \, K(q_F, t_F; q_0, t_0) K(q_F', t_F'; q_0', t_0')(\psi(q_0, t_0)\phi(q_0', t_0')) \tag{2.5}$$

$$= \int \mathrm{d}q_0 \, K(q_F, t_F; q_0, t_0)\psi(q_0, t_0) \int \mathrm{d}q_0' \, K(q_F', t_F'; q_0', t_0')\phi(q_0', t_0'), \tag{2.6}$$

eq. (2.4) says that $\langle q_F, q_F' | \eta(t_F) \rangle$ is the product of the probability that ψ is at (q_F, t_F), and (q_F', t_F'). Therefore, $\langle q_F, q_F' | \eta(t_F) \rangle$ represents the joint probability distribution of the two states, and it can be found via the product of propagators,

$$K(q_F, t_F; q_0, t_0) K(q_F', t_F'; q_0', t_0'). \tag{2.7}$$

2.1.2 Interacting systems

Let there be a state ket $|\eta\rangle$ which describes the quantum state of two particles. When the two particles are interacting, the time-evolution operator cannot be factored into tensor products of two operators. Therefore, there can only be one combined time-evolution operator for both of the systems:

$$\hat{U}(t_F, t_0) = \exp\left[-\mathrm{i}\Delta t \left(\frac{\hat{p}^2}{2m} + \frac{\hat{p}'^2}{2m'} + V(\hat{q}, \hat{q}', t)\right)\right] \tag{2.8}$$

The consequence of the combined time-evolution operator is that, we cannot calculate the joint probability distribution between different time of the subsystem. For simplicity' sake, let the index $j = i + 1$, where $t_j = t_i + \Delta t$ in which $\Delta t \to 0$.

$$\left\langle q_j, q_j' \middle| \eta(t_j) \right\rangle \tag{2.9}$$

$$= \left\langle q_j, q_j' \middle| \hat{U}(t_j, t_i) \middle| \eta(t_i) \right\rangle . \tag{2.10}$$

$$= \iint \mathrm{d}q_i \, \mathrm{d}q_i' \left\langle q_j, q_j' \middle| \hat{U}(t_j, t_i) \middle| q_i, q_i' \right\rangle \left\langle q_i, q_i' | \eta(t_i) \right\rangle . \tag{2.11}$$

As seen, the form of transition element is

$$\left\langle q_j, q_j' \middle| \exp\left[-\mathrm{i}\Delta t \left(\frac{\hat{p}^2}{2m} + \frac{\hat{p}'^2}{2m'} + V(\hat{q}, \hat{q}', t)\right)\right] \middle| q_i, q_i' \right\rangle . \tag{2.12}$$

The terms in the exponents can be separated due to the vanishing commutator when $\Delta t \to 0$. By separating the terms in the exponents and inserting two complete sets of momentum basis, the

equation above turns into

$$\frac{1}{(2\pi)^2}\iint \mathrm{d}p\,\mathrm{d}p'\,\left\langle q_j,q_j'\left|\exp\left[-\mathrm{i}\Delta t\frac{\hat{p}^2}{2m}\right]\right|p,p'\right\rangle \left\langle p,p'|\exp\left[-\mathrm{i}\Delta t\frac{\hat{p}'^2}{2m'}\right]\exp\left[-\mathrm{i}\Delta t V(\hat{q},\hat{q}',t)\right]|q_i,q_i'\right\rangle$$

$$=\frac{1}{(2\pi)^2}\iint \mathrm{d}p\,\mathrm{d}p'\exp\left[-\mathrm{i}u\Delta t\left(\frac{p^2}{2m}+\frac{p'^2}{2m'}+V(q_i,q_i,\Delta t)\right)\right]\langle q_j|p\rangle\left\langle q_j'\big|p'\right\rangle\langle q_i|p\rangle^*\left\langle q_j'\big|p'\right\rangle^*$$

$$=\frac{1}{(2\pi)^4}\mathrm{e}^{-\mathrm{i}\Delta t V(q_i,q_i',t)}\int \mathrm{d}p\exp\left[-\mathrm{i}\Delta t\frac{p^2}{2m}+\mathrm{i}p(q_j-q_i)\right]\int \mathrm{d}p'\exp\left[-\mathrm{i}\Delta t\frac{p'^2}{2m'}+\mathrm{i}p'(q_j'-q_i')^2\right]$$

$$=\frac{(mm')^{\frac{1}{2}}}{8\pi^3\mathrm{i}\Delta t}\exp\left[-\mathrm{i}\Delta t V(q_i,q_i',t)+\frac{\mathrm{i}m'}{2\Delta t}(q_j'-q_i')^2+\frac{\mathrm{i}m}{2\Delta t}(q_j-q_i)^2\right].\tag{2.13}$$

To find the propagator for an interacting system, we need to perform successive integrals on q and q', i.e.,

$$K_\eta=\int\cdots\int \mathrm{d}q_N\,\mathrm{d}q_N'\ldots \mathrm{d}q_1\,\mathrm{d}q_1'\,\left\langle q_F,q_F'|\hat{U}(t_F,t_N)|q_N,q_N'\right\rangle\ldots\left\langle q_1,q_1'|\hat{U}(t_1,t_0)|q_0,q_0'\right\rangle\tag{2.14}$$

Notice that when there is no interaction between the two systems ($V=0$), the integrals become separable and reduces down to the form of the non-interacting system's propagator but off by a normalization factor.

There are two common forms of interaction, which is the spring interaction and the coulomb interaction. Both of which includes the term $(q_i-q_i')^2$ in $V(q,q')$, which causes major problems in integration. When expanded, there is a q_iq_i' term that makes the integral inseparable which causes the integral pattern to not repeat; therefore, we resort to perturbation.

2.2 Form of the two particle perturbation series

The perturbation series for one particle are already given by Feynman in his path integrals textbook:

$$K_n(F,0)=(-\mathrm{i})^n\int\cdots\int K_0(F,n)\prod_{i=1}^{n}V(i)K(i,i-1)\,\mathrm{d}\tau_i\tag{2.15}$$

where $K(j,k)=K(q_j,t_j;q_k,t_k)$. To apply it with two particles, we extend it:

$$K_n(F,0;F',0')=(-\mathrm{i})^n\int\cdots\int K_0(F,n)K_0(F',n')\left[\prod_{i=1}^{n}V(i)K(i,i-1)K(i',i-1')\,\mathrm{d}q_i\,\mathrm{d}q_i'\right]\mathrm{d}t\,.\tag{2.16}$$

where $K=\Sigma\,K_n$. For some potential, it is possible to evaluate this series term by term analytically using the Meijer's G function.

2.3 The spring system

The spring potential is given by $V(q,q')=k/2\,(q-q')^2$, which I shall let $\alpha=k/2$ for simplicity sake.

2.3.1 First order perturbation term

From eq. (2.16), set $t_1 = t, t_0 = 0$

$$K_1(F, 0; F', 0)$$

$$= (-\mathrm{i})^1 \iiint K_0(F, 1) K_0(F', 1') K_0(1, 0) K_0(1, 0') \alpha (q_1 - q_1')^2 \, \mathrm{d}q_1 \, \mathrm{d}q_1' \, \mathrm{d}t . \tag{2.17}$$

$$= -\mathrm{i}\alpha \int_0^{t_F} \left[\iint K_0(q_F, q_1; t_F - t) K_0(q_F', q_1'; t_F - t) K_0(q_1, q_0; t) K_0(q_1', q_0'; t) (q_1 - q_1')^2 \, \mathrm{d}q_1 \, \mathrm{d}q_1' \right] \mathrm{d}t .$$

We then let the terms in the square bracket,

$$\iint K_0(q_F, q_1; t_F - t) K_0(q_F', q_1'; t_F - t) K_0(q_1, q_0; t) K_0(q_1', q_0'; t) (q_1 - q_1')^2 \, \mathrm{d}q_1 \, \mathrm{d}q_1' \tag{2.18}$$

equals I; therefore, $K_1 = -\mathrm{i}\alpha \int_0^{t_F} I \, \mathrm{d}t$.

We then separate I into three integrals:

$$I_{P1} = \int q_1^2 K_0(q_F, q_1; t_F - t) K_0(q_1, q_0; t) \, \mathrm{d}q_1 \int K_0(q_F', q_1'; t_F, t) K_0(q_1', q_0'; t) \, \mathrm{d}q_1' , \tag{2.19}$$

$$I_{P2} = \int K_0(q_F, q_1; t_F - t) K_0(q_1, q_0; t) \int q_1'^2 K_0(q_F', q_1'; t_F, t) K_0(q_1', q_0'; t) \, \mathrm{d}q_1' , \tag{2.20}$$

$$I_{P3} = \int q_1 K_0(q_F, q_1; t_F - t) K_0(q_1, q_0; t) \int q_1' K_0(q_F', q_1'; t_F, t) K_0(q_1', q_0'; t) \, \mathrm{d}q_1' , \tag{2.21}$$

where $I = I_{P1} + I_{P2} + 2I_{P3}$. The integrals without the factor q_1 and q_1^2 can be reduced into the kernel for the free particle:

$$I_{P1} = K_0(q_F', q_0'; t_F) \int q_1^2 K_0(q_F, q_1; t_F - t) K_0(q_1, q_0; t) \, \mathrm{d}q_1 \tag{2.22}$$

$$I_{P2} = K_0(q_F, q_0; t_F) \int q_1'^2 K_0(q_F', q_1'; t_F - t) K_0(q_1', q_0'; t) \, \mathrm{d}q_1' \tag{2.23}$$

Since I_{P2} can be obtained by switching all the primed variables with the corresponding unprimed in I_{P1}, we're left with two family of integrals:

$$\int q_1 K_0(q_F, q_1; t_F - t) K_0(q_1, q_0; t) \, \mathrm{d}q_1 \quad \text{and,} \quad \int q_1 K_0(q_F, q_1; t_F - t) K_0(q_1, q_0; t) \, \mathrm{d}q_1 . \tag{2.24}$$

To evaluate these, we first simplify the product of kernel under the assumption that $t_F > t$.

$$K_0(q_F, q_1; t_F - t) K_0(q_1, q_0; t)$$

$$= \sqrt{\frac{m}{2\pi \mathrm{i}(t_F - t)}} \sqrt{\frac{m}{2\pi \mathrm{i}t}} \exp\left[-\frac{\mathrm{i}m}{2(t_F - t)}(q_F - q_1)^2 - \frac{\mathrm{i}m}{2t}(q_1 - q_0)^2 \right] \tag{2.25}$$

$$= \frac{m}{2\pi} \sqrt{-\frac{1}{t(t_F - t)}} \exp\left[q_1^2 \left(\frac{\mathrm{i}m}{2t} + \frac{\mathrm{i}m}{2(t_F - t)} \right) - q_1 \left(\frac{\mathrm{i}mq_0}{t} + \frac{\mathrm{i}mq_F}{t_F - t} \right) + \left(\frac{\mathrm{i}mq_0^2}{2t} + \frac{\mathrm{i}mq_F^2}{2(t_F - t)} \right) \right]$$

$$= \frac{m}{2\pi} \sqrt{-\frac{1}{t(t_F - t)}} \exp\left[-q_1^2 \left(\frac{mt_F}{2\mathrm{i}t(t_F - t)} \right) - q_1(\mathrm{i}m) \left(\frac{q_0}{t} + \frac{q_F}{t_F - t} \right) - \left(\frac{m}{2\mathrm{i}} \right) \left(\frac{q_0^2}{t} + \frac{q_F^2}{t_F - t} \right) \right]$$

The normalization factor are pulled out. Both integrals in eq. (2.24) can be evaluated with

$$a = \frac{mt_F}{2it(t_F - t)}, \quad b = im\left(\frac{q_0}{t} + \frac{q_F}{t_F - t}\right) \quad \text{and,} \quad c = \left(\frac{m}{2i}\right)\left(\frac{q_0^2}{t} + \frac{q_F^2}{t_F - t}\right) \tag{2.26}$$

in which,

$$\exp\left[\frac{b^2}{4a} - c\right] = \exp\left[\frac{im}{2t_F}(q_F - q_0)^2\right] = \sqrt{\frac{2\pi it_F}{m}}K_0(q_F, q_0; t_F). \tag{2.27}$$

To summarize,

$$\int q_1 K_0(q_F, q_1; t_F - t)K_0(q_1, q_0; t)\,dq_1 = -\frac{b}{2}\sqrt{\frac{\pi}{a^3}} \times \frac{m}{2\pi}\sqrt{-\frac{1}{t(t_F - t)}} \times \sqrt{\frac{2\pi it_F}{m}}K_0(q_F, q_0; t_F)$$

$$= -\frac{b}{2}\sqrt{\frac{\pi}{a^3}} \times \sqrt{\frac{mt_F}{2\pi it(t_F - t)}}K_0(q_F, q_0; t_F), \tag{2.28}$$

and

$$\int q_1^2 K_0(q_F, q_1; t_F - t)K_0(q_1, q_0; t)\,dq_1 = \frac{1}{4}\sqrt{\frac{\pi}{a^5}}(2a + b^2) \times \sqrt{\frac{mt_F}{2\pi it(t_F - t)}}K_0(q_F, q_0; t_F). \tag{2.29}$$

On the Gaussian integral with degree one,

$$-\frac{b}{2}\sqrt{\frac{\pi}{a^3}} = \sqrt{\frac{2\pi t}{mt_F^3}}\frac{\sqrt{-i(t_F - t)^3}}{i(t_F - t)} \times [q_0(t_F - t) + q_F t]; \tag{2.30}$$

thus from eq. (2.28),

$$\int q_1 K_0(q_F, q_1; t_F - t)K_0(q_1, q_0; t) = \sqrt{\frac{2\pi t}{mt_F^3}}\frac{\sqrt{-i(t_F - t)^3}}{i(t_F - t)} \times [q_0(t_F - t) + q_F t] \tag{2.31}$$

$$\times \sqrt{\frac{mt_F}{2\pi it(t_F - t)}}K_0(q_F, q_0; t_F)$$

$$= -\frac{1}{t_F}[q_0(t_F - t) + q_F t]K_0(q_F, q_0; t_F). \tag{2.32}$$

On the Gaussian integral with degree two,

$$\frac{1}{4}\sqrt{\frac{\pi}{a^5}}(2a + b^2) = -\sqrt{\frac{2\pi t}{m^3 t_F^5}}\frac{\sqrt{i(t_F - t)^5}}{(t_F - t)^2}\left[m\left(q_0(t_F - t) + q_F t\right)^2 + itt_F(t_F - t)\right]; \tag{2.33}$$

and thus,

$$\int q_1^2 K_0(q_F, q_1; t_F - t)K_0(q_1, q_0; t)\,dq_1 \tag{2.34}$$

$$= \sqrt{\frac{mt_F}{2\pi it(t_F - t)}}K_0(q_F, q_0; t_F) \times -\sqrt{\frac{2\pi t}{m^3 t_F^5}}\frac{\sqrt{i(t_F - t)^5}}{(t_F - t)^2}\left[m\left(q_0(t_F - t) + q_F t\right)^2 + itt_F(t_F - t)\right]$$

$$= -\frac{1}{mt_F^2}\left[m\left(q_0(t_F - t) + q_F t\right)^2 + itt_F(t_F - t)\right]K_0(q_F, q_0; t_F). \tag{2.35}$$

We're now in the place to finally construct the first order propagator term for the spring system. Recall that

$$K_1 = -i\alpha\int_0^{t_F} I\,dt = -i\alpha\left[\int_0^{t_F} I_{P1}\,dt + \int_0^{t_F} I_{P2}\,dt + 2\int_0^{t_F} I_{P3}\,dt\right] \tag{2.36}$$

From earlier,

$$
\begin{aligned}
I_{P1} &= K_0(q_F', q_0'; t_F) \int q_1^2 K_0(q_F, q_1; t_F - t) K_0(q_1, q_0; t)\, dq_1 \\
&= -\frac{1}{m t_F^2} \left[m \left(q_0(t_F - t) + q_F t \right)^2 + i t t_F (t_F - t) \right] K_0(q_F, q_0; t_F) K_0(q_F', q_0'; t_F),
\end{aligned}
\tag{2.37}
$$

$$
\begin{aligned}
I_{P2} &= K_0(q_F, q_0; t_F) \int q_1'^2 K_0(q_F', q_1'; t_F - t) K_0(q_1', q_0'; t)\, dq_1' \\
&= -\frac{1}{m t_F^2} \left[m \left(q_0'(t_F - t) + q_F' t \right)^2 + i t t_F (t_F - t) \right] K_0(q_F, q_0; t_F) K_0(q_F', q_0'; t_F),
\end{aligned}
\tag{2.38}
$$

$$
\begin{aligned}
I_{P3} &= -\frac{1}{t_F} \left[q_0(t_F - t) + q_F t \right] K_0(q_F, q_0; t_F) \times -\frac{1}{t_F} \left[q_0'(t_F - t) + q_F' t \right] K_0(q_F', q_0'; t_F) \\
&= \frac{1}{t_F^2} \left[q_0(t_F - t) + q_F t \right] \left[q_0'(t_F - t) + q_F' t \right] K_0(q_F, q_0; t_F) K_0(q_F', q_0'; t_F).
\end{aligned}
\tag{2.39}
$$

Thus,

$$
\begin{aligned}
K_1 = -i\alpha K_0(q_F, q_0; t_F) K_0(q_F', q_0'; t_F) \frac{1}{t_F^2} \Bigg[&-\frac{1}{m} \int_0^{t_F} m \left(q_0(t_F - t) + q_F t \right)^2 + i t t_F (t_F - t)\, dt \\
&- \frac{1}{m} \int_0^{t_F} m \left(q_0'(t_F - t) + q_F' t \right)^2 + i t t_F (t_F - t)\, dt \\
&+ \int_0^{t_F} \left[q_0(t_F - t) + q_F t \right] \left[q_0'(t_F - t) + q_F' t \right] dt \Bigg]
\end{aligned}
\tag{2.40}
$$

The integrals are then taken out to be evaluated term by term. Since the integrand of these integrals are all polynomials, we can just plug it into `SymPy.jl`:

$$
\int_0^{t_F} m \left(q_0(t_F - t) + q_F t \right)^2 = \frac{t_F^3}{6} \left(2m(q_0 + q_F)^2 + i t_F \right)
\tag{2.41}
$$

$$
\int_0^{t_F} m \left(q_0'(t_F - t) + q_F' t \right)^2 = \frac{t_F^3}{6} \left(2m(q_0' + q_F')^2 + i t_F \right)
\tag{2.42}
$$

$$
\int_0^{t_F} \left[q_0(t_F - t) + q_F t \right] \left[q_0'(t_F - t) + q_F' t \right] dt = \frac{t_F^3}{6} \left(2q_0 q_0' + q_0 q_F' + q_0' q_F + 2 q_F q_F' \right)
\tag{2.43}
$$

Therefore, the first order perturbation term of the spring system takes the form

$$
\begin{aligned}
K_1(q_F, q_0; q_F', q_0'; t_F) = -i\frac{\alpha t_F}{6} K_0(q_F, q_0; t_F) K_0(q_F', q_0'; t_F) \\
\times \left[-2 \left(m(q_0 + q_F)^2 + m(q_0' + q_F')^2 + i t_F \right) + 2 q_0 q_0' + q_0 q_F' + q_0' q_F + 2 q_F q_F' \right].
\end{aligned}
\tag{2.44}
$$

2.3.2 Second order perturbation term

The second order perturbation term, K_2 is

$$
K_2 = \int \cdots \int K_0(F, 2) V(2) K_0(2, 1) V(1) K_0(1, 0)\, dq_1\, dq_1'\, dt_1\, dq_2\, dq_2'\, dt_2
\tag{2.45}
$$

$$
= \int \cdots \int K_0(q_F, q_2; t_F - t_2) K_0(q_F', q_2'; t_F - t_2) K_0(q_2, q_1; t_2 - t_1) K_0(q_2', q_1'; t_2 - t_1)
\tag{2.46}
$$

$$
\times K_0(q_1, q_0; t_1 - t_0) K_0(q_1', q_0'; t_1 - t_0)(q_2 - q_2')^2 (q_1 - q_1')^2\, dq_1\, dq_1'\, dt_1\, dq_2\, dq_2'\, dt_2
$$

$$
= \int_{t_1}^{t_F} \int_{t_0}^{t_F} \left[\int \cdots \int K_0(q_F, q_2; t_F - t_2) K_0(q_F', q_2'; t_F - t_2) K_0(q_2, q_1; t_2 - t_1) \right. \tag{2.47}
$$

$$
\times K_0(q_2, q_1; t_2 - t_1) K_0(q_1, q_0; t_1 - t_0) K_0(q_1, q_0; t_1 - t_0) \left(q_1^2 q_2^2 - 2q_1^2 q_2 q_2' \right.
$$

$$
+ q_1^2 \left(q_2' \right)^2 - 2q_1 q_2^2 q_1' + 4q_1 q_2 q_1' q_2' - 2q_1 q_1' \left(q_2' \right)^2 + q_2^2 \left(q_1' \right)^2
$$

$$
\left. \left. -2q_2 \left(q_1' \right)^2 q_2' + \left(q_1' \right)^2 \left(q_2' \right)^2 \right) \mathrm{d}q_1 \, \mathrm{d}q_1' \, \mathrm{d}q_2 \, \mathrm{d}q_2' \right] \mathrm{d}t_1 \, \mathrm{d}t_2
$$

The integral once again can be broken into nine integrals that must be integrated w.r.t. time twice later on. All those nine integrals have a product of propagator as a multiplier. We shall evaluate those first, separating the primed and unprimed variables.

$$
K_0(q_F, q_2; t_F - t_2) K_0(q_F', q_2'; t_F - t_2) K_0(q_2, q_1; t_2 - t_1) K_0(q_2, q_1; t_2 - t_1) K_0(q_1, q_0; t_1 - t_0)
$$

$$
\times K_0(q_1, q_0; t_1 - t_0)
$$

$$
= \frac{im^3}{8\pi^3 (t_F - t_2)(t_2 - t_1)(t_1 - t_0)} \exp \left[\frac{im}{2(t_F - t_2)} \left((q_F - q_2)^2 + (q_F' - q_2')^2 \right) \right. \tag{2.48}
$$

$$
\left. + \frac{im}{2(t_2 - t_1)} \left((q_2 - q_1)^2 + (q_2' - q_1')^2 \right) + \frac{im}{2(t_1 - t_0)} \left((q_1 - q_0)^2 + (q_1' - q_0')^2 \right) \right]
$$

2.3.3 The joint probability distribution

2.4 The delta function collision problem

The potential for the delta function collision problem is

$$
V = V_0 \delta(q - q') \tag{2.49}
$$

where V_0 is the strength of the delta function, and is generally considered to be negative.

2.4.1 First order perturbation term

We evaluate the perturbation term similarly to how we did it in section 2.3.1, starting with the form:

$$
K_1(F, 0; F', 0) \tag{2.50}
$$

$$
= -i \int_0^{t_F} \left[\iint K_0(q_F, q_1; t_F - t) K_0(q_F', q_1'; t_F - t) K_0(q_1, q_0; t) K_0(q_1', q_0'; t) V_0 \delta(q_1 - q_1') \, \mathrm{d}q_1 \, \mathrm{d}q_1' \right] \mathrm{d}t.
$$

$$
= -iV_0 \int_0^{t_F} \left[\iint K_0(q_F, q_1; t_F - t) K_0(q_F', q_1'; t_F - t) K_0(q_1, q_0; t) K_0(q_1', q_0'; t) \delta(q_1 - q_1') \, \mathrm{d}q_1 \, \mathrm{d}q_1' \right] \mathrm{d}t
$$

Let I_1 represents the integral in the square bracket; thus, $K_1 = -iV_0 \int_0^{t_F} I_1 \, \mathrm{d}t$. Then,

$$
I_1 = \iint K_0(q_F, q_1; t_F - t) K_0(q_F', q_1'; t_F - t) K_0(q_1, q_0; t) K_0(q_1', q_0'; t) \delta(q_1 - q_1') \, \mathrm{d}q_1 \, \mathrm{d}q_1' \tag{2.51}
$$

$$
= \int K_0(q_F, q_1'; t_F - t) K_0(q_F', q_1'; t_F - t) K_0(q_1', q_0; t) K_0(q_1', q_0'; t) \, \mathrm{d}q_1' \tag{2.52}
$$

2.5 The coulomb problem

Implementation of simulations

To represent the joint probability distribution of a two particle system, we need four axes. Two for the position of each Hilbert space that those particles belong in, one for the probability amplitude, and one for the time.

$$P(q_F, q_F'; t_F) = |\langle q_F, q_F'|\eta(t_F)\rangle|^2 \tag{3.1}$$

$$= \left| \iint K(q_F, q_F', t_F; q_0, q_0', t_0)\eta(q_0, q_0', t_0) \, \mathrm{d}q_0 \, \mathrm{d}q_0' \right|^2 \tag{3.2}$$

$$= \left| \iint \left\{ \sum_{i=0}^{\infty} K_i(q_F, q_F', t_F; q_0, q_0', t_0) \right\} \eta(q_0, q_0', t_0) \, \mathrm{d}q_0 \, \mathrm{d}q_0' \right|^2 \tag{3.3}$$

For this equation to work with a discrete simulation, we need to exchange the integral sign with the summation sign:

$$= \left| \sum_{q_0} \sum_{q_0'} \left\{ \sum_{i=0}^{\infty} K_i(q_F, q_F', t_F; q_0, q_0', t_0) \right\} \eta(q_0, q_0', t_0) \right| \tag{3.4}$$

The sum of propagators can then be truncated to our liking. I've written the code in `Julia` to test for the free particle propagator, and it looks something like this:

```julia
using Plots; plotlyjs()
using LinearAlgebra
using SymPy
using BenchmarkTools

q, q0, q1, q2, qf = symbols("q q_0 q_1 q_2 q_F", real = true)
m, t, t0, t1, t2, tf = symbols("m t t_0 t_1 t_2 t_F", real = true, positive = true)
q0p, q1p, q2p, qfp = symbols("q^{\\prime}_0 q^{\\prime}_1 q^{\\prime}_2 q^{\\prime}_F",
    real = true)
```

```julia
a, b, c, d, e, f = symbols("a b c d e f")
s1, s2, p1, p2, σ1, σ2 = symbols("s_1 s_2 p_1 p_2 σ_1 σ_2")

freePropagator(finPos, startPos, finTime, startTime = 0, m = 1) = sqrt(m / (2 * pi * im *
↪ (finTime - startTime))) * exp(im * m / (2 * (finTime - startTime)) * (finPos -
↪ startPos)^2)
freePropagatorC(qf, qfp, q0, q0p, tf, t0) = freePropagator(qf, q0, tf, t0) +
↪ freePropagator(qfp, q0p, tf, t0)

initStateFunction(q0, q0p, σ1, s1, p1, σ2, s2, p2) = (1//2 * pi * σ1)^(1//4) * exp(-(q0 -
↪ s1)^2 / (4 * σ1^2) + im * p1 * q0) * (1//2 * pi * σ2)^(1//4) * exp(-(q0p - s2)^2 / (4 *
↪ σ2^2) + im * p2 * q0p)

maxPos = 5
minPos = -5
stepPos = 0.25

pos1Vect = collect(minPos:stepPos:maxPos)
pos2Vect = collect(minPos:stepPos:maxPos)
posVectSize = size(pos1Vect, 1)
posMat = [(i, j) for i in pos1Vect, j in pos2Vect]

posToIndex(pos) = Int32((pos - minPos) / stepPos  + 1)

initState(q) = initStateFunction(q[1], q[2], 1, 2, 2, 1, -2, -2)
initMat = initState.(posMat)
initMat = round.(initMat, digits = 7)

surface(pos1Vect, pos2Vect, abs.(initMat))

finalTime = 1
finalMat = Matrix{ComplexF32}(undef, posVectSize, posVectSize)

for xf in pos1Vect, xfp in pos2Vect
    sumPos = 0
    for i in 1:posVectSize, j in 1:posVectSize
```

```
40        x0 = pos1Vect[i]
41        x0p = pos2Vect[j]
42        sumPos += freePropagatorC(xf, xfp, x0, x0p, finalTime, 0) * initMat[i, j]
43      end
44    finalMat[posToIndex(xf), posToIndex(xfp)] = sumPos
45  end
46
47  surface(pos1Vect, pos2Vect, abs2.(finalMat))
```

The Schrödinger's equation for two particles

Integrals evaluation code

All of these codes that I've written are in the `Julia` language, which I've imported three packages: `Sympy`, `OffsetArrays`, and `Plots; plotlyjs()`

A.1 Polynomial extraction

Since we're going to be doing a lot of polynomials rearranging, I've implemented the polynomial extraction function as follows:

```julia
function extractPolynomial(expr, arg)
    expr isa Sym ? nothing : expr = sympify(1)
    expr = expand(expr)
    polyDegree = Int(degree(expr, arg))
    extractOneSet = []
    for i in 0:polyDegree
        temp = expr.coeff(arg, i)
        push!(extractOneSet, temp)
    end
    polyExt = OffsetVector(extractOneSet, 0:polyDegree)
    return polyExt
end
```

This function accepts two arguments: `expr`, which is the expression you want to extract, and `arg`, the variable that you extract with respect to. For example, inputting $ax^2 + bx + c$, x would give

out

$$
\begin{bmatrix} a \\ b \\ c \end{bmatrix},
\tag{A.1}
$$

which is a zero index matrix.

A.2 Code for the spring problem

A.2.1 First order perturbation

The first order perturbation uses the following symbols:

```
1   @syms q0 q1 q2
2   @syms m::(real, positive) t::(real, positive)
3   q0', q1', q2', qf', qf = symbols("q_{0}^{\\prime}, q_{1}^{\\prime}, q_{2}^{\\prime},
    ↪  q_{F}^{\\prime}, q_F")
4   t0, t1, t2, tf = symbols("t_0, t_1, t_2, t_F", real = true, positive = true)
```

The following code is used to aid the evaluation of integrals.

```
1   # Simplifying the product of propagators in eq. 2.25
2   idenFunc = IM*m/(2 * (tf - t)) * (qf - q1)^2 + IM*m/(2*t) * (q1 - q0)^2
3
4   idenPoly = extractPolynomial(idenFunc, q1)
5   idenPolyA = -idenPoly[2]
6   idenPolyB = -idenPoly[1]
7   idenPolyC = -idenPoly[0]
8
9   display(idenPolyA)
10  display(idenPolyB)
11  display(idenPolyC)
12
```