Quantum harmonic oscillator revisited: A Fourier transform approach

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NOTES AND DISCUSSIONS

An elementary derivation of the harmonic oscillator propagator

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The harmonic oscillator propagator is found straightforwardly from the free particle propagator within the imaginary-time Feynman path integral formalism. The derivation is simple, and requires only elementary mathematical manipulations and no clever use of Hermite polynomials, annihilation and creation operators, cumbersome determinant evaluations, or involved algebra.
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Many believe that the evaluation of the simple harmonic oscillator propagator is tricky. Previous arguments[1–5] confirm this belief to a certain extent. The aim of this note is to present an alternative and simple derivation of the imaginary time harmonic oscillator propagator[1] (known as the harmonic oscillator density matrix in the statistical physics context),

$$Z_{\mathrm{HO}} = \int Dx \exp\left(-\int_0^T dt \left(\frac{m}{2}\dot{x}^2 + \frac{m\omega^2}{2}x^2 \right)\right). \tag{1}$$

All one needs to know to follow the proof is the standard expression for the imaginary-time free particle propagator,[1]

$$Z_{\mathrm{FP}} = \int Dx \exp\left(-\int_0^T dt \frac{m}{2}\dot{x}^2 \right) = \sqrt{\frac{m}{2\pi T}} \exp\left(-\frac{m}{2T}(x_T - x_0)^2 \right), \tag{2}$$

where the functional integration measure is defined as

$$Dx \equiv \lim_{\epsilon_i \to 0} \sqrt{\frac{m}{2\pi\epsilon_N}} \prod_{i=1}^{N-1} \sqrt{\frac{m}{2\pi\epsilon_i}} dx_i . \tag{3}$$

The time interval T in Eq. (3) has been sliced into N pieces, not necessarily equally, with sizes $\epsilon_i \equiv t_i - t_{i-1}$.

Observe that Eq. (1) can be rewritten as

$$Z_{\mathrm{HO}} = \int Dx \exp\left[-\int_0^T dt \left(\frac{m}{2}(\dot{x}+\omega x)^2 - \frac{m\omega}{2}\frac{dx^2}{dt} \right)\right] = \exp\left(\frac{m\omega}{2}(x_T^2 - x_0^2) \right) \int Dx \exp\left(-\int_0^T dt \frac{m}{2}(\dot{x}+\omega x)^2 \right). \tag{4}$$

If we substitute $x(t) \equiv z(t)\exp(-\omega t)$ in Eq. (4), we obtain

$$Z_{\mathrm{HO}} = \exp\left(\frac{m\omega}{2}(x_T^2 - x_0^2) \right) \left(\prod_{i=1}^{N-1} \exp(-\omega t_i) \right) \times \int Dz \exp\left(-\int_0^T dt \frac{m}{2}\exp(-2\omega t)\dot{z}^2 \right). \tag{5}$$

The exponential factor $\exp(-2\omega t)$ in Eq. (5) can be absorbed by time reparametrization. Let $t^* \equiv \exp(2\omega t)/2\omega + c$, where c is an unimportant arbitrary constant. From Eq. (5), we have

$$Z_{\mathrm{HO}} = \exp\left(\frac{m\omega}{2}(x_T^2 - x_0^2) + \frac{\omega T}{2} \right) \times \int Dz^* \exp\left(-\int_{t_a}^{t_b} dt^* \frac{m}{2}(\dot{z}^*)^2 \right), \tag{6}$$

where $z^*(t^*) = z(t)$, $t_a = 1/2\,\omega + c$, and $t_b = \exp(2\omega T)/2\omega + c$. To obtain Eq. (6), it is necessary to take into account that $\epsilon_i^* \equiv t_i^* - t_{i-1}^* = [\exp(2\omega t_i) - \exp(2\omega t_{i-1})]/2\omega = \epsilon_i \exp(2\omega\bar{t}_i)$, where $\bar{t}_i \equiv (t_i + t_{i-1})/2$, (Ref. 6) so that

$$\begin{aligned}\left(\prod_{i=1}^{N-1} \exp(-\omega t_i) \right) Dz &\equiv \sqrt{\frac{m}{2\pi\epsilon_N}} \prod_{i=1}^{N-1} \exp(-\omega t_i) \sqrt{\frac{m}{2\pi\epsilon_i}} dz_i \\ &= \exp\left(\frac{\omega T}{2} \right) \sqrt{\frac{m}{2\pi\epsilon_N \exp(2\omega\bar{t}_N)}} \prod_{i=1}^{N-1} \times \sqrt{\frac{m}{2\pi\epsilon_i \exp(2\omega\bar{t}_i)}} dz_i \\ &= \exp\left(\frac{\omega T}{2} \right) \sqrt{\frac{m}{2\pi\epsilon_N^*}} \prod_{i=1}^{N-1} \sqrt{\frac{m}{2\pi\epsilon_i^*}} dz_i^* \\ &= \exp\left(\frac{\omega T}{2} \right) Dz^*. \end{aligned} \tag{7}$$

If we substitute the free particle expression (2) into Eq. (6) and use the definitions of t_a, t_b, and $z^*(t^*)$, we obtain

$$Z_{\mathrm{HO}}=\exp\left(\frac{m\omega}{2}(x_T^2-x_0^2)+\frac{\omega T}{2}\right)\sqrt{\frac{m}{2\pi(t_b-t_a)}}$$
$$\times\exp\left(-\frac{m}{2(t_b-t_a)}(z_{t_b}^*-z_{t_a}^*)^2\right)$$
$$=\sqrt{\frac{m\omega}{2\pi\sinh(\omega T)}}\exp\left(-\frac{m\omega}{2\sinh(\omega T)}[(x_T^2+x_0^2)\right.$$
$$\left.\times\cosh(\omega T)-2x_Tx_0]\right), \tag{8}$$

which is the well-known expression for the imaginary-time harmonic oscillator propagator.[1] The quantum mechanical propagator can be immediately found from Eq. (8) by the analytical mapping $T\to iT$.[1]

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[1]R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965), pp. 71–73 and 273–279.
[2]J. J. Sakurai, *Modern Quantum Mechanics* (Addison-Wesley, Redwood City, CA, 1985), pp. 109–123.
[3]B. R. Holstein, ‘‘The harmonic oscillator propagator,’’ Am. J. Phys. **66**, 583–589 (1998).
[4]F. A. Barone and C. Farina, ‘‘The zeta function method and the harmonic oscillator propagator,’’ Am. J. Phys. **69**, 232–235 (2001).
[5]F. A. Barone, H. Boschi-Filho, and C. Farina, ‘‘Three methods for calculating the Feynman propagator,’’ Am. J. Phys. **71**, 483–491 (2003).
[6]The choice $\overline{t_i}=(t_i+t_{i-1})/2$ is the only prescription that leads to a time translational invariant propagator.

Quantum harmonic oscillator revisited: A Fourier transform approach

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I present a Fourier transform approach to the problem of finding the stationary states of a quantum harmonic oscillator. The simplicity of the method may make it a desirable substitute for the rather cumbersome polynomial approach to the problem which is commonly used in the standard graduate quantum mechanics textbooks.
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The quantum harmonic oscillator is one of the most ubiquitous models in physics. Quantum oscillator models play a prominent role in many branches of physics including quantum optics and solid state theory, to mention but a few examples. One of the most important characteristics of a one-dimensional harmonic oscillator is its energy eigenstates, which can be described in terms of their coordinate space wave functions $\psi_n(x)$:[1,2]

$$\frac{d^2\psi_n}{dX^2}+\frac{2M}{\hbar^2}\left(E_n-\frac{M\Omega^2X^2}{2}\right)\psi_n=0. \tag{1}$$

Here X is a spatial coordinate, E_n is the energy of the nth stationary state (eigenstate) of the oscillator, and M and Ω are the mass and the frequency of the oscillator, respectively.

In many quantum mechanics textbooks[1,2] Eq. (1) is solved with the help of the Sommerfeld polynomial approach.[3] Not only is the latter unwieldy, but it often makes the student wonder about the ‘‘magical’’ way the corresponding series solution terminates only for certain integer values of the energy.[4] Of course, there exists an alternative algebraic approach (see, for example, Ref. 5) which is free from this shortcoming, but it requires familiarity with operator algebra in Fock space.

In this note, I present yet another approach to the same problem that relies on a simple Fourier transformation. Besides its simplicity, the proposed method provides a useful link between the material that students typically learn in a course on mathematical physics and an important physical problem.

I begin by introducing the dimensionless variables: $\epsilon=E_n/\hbar\Omega$ and $x=X/l_0$, where $l_0=(\hbar/M\Omega)^{1/2}$ is a characteristic spatial scale associated with the ground state wave function of the oscillator. Equation (1) can then be written in the form

$$\frac{d^2\psi}{dx^2}+(2\epsilon-x^2)\psi=0, \tag{2}$$

where I have omitted, for brevity, the subscript n on the wave function. It is readily seen from Eq. (2) that if $\psi(x)$ is a solution, so is $\psi(-x)$. Consequently, the wave functions describing the stationary states can be chosen to be either even or odd. I will assume in the following that all eigenfunctions have a definite parity.

By substituting $\psi(x)=\phi(x)e^{x^2/2}$ into Eq. (2), I obtain

$$\phi''+2x\phi'+(2\epsilon+1)\phi=0, \tag{3}$$

where the prime denotes a derivative with respect to x. In order to solve Eq. (3), I consider a Fourier transform of ϕ:

$$\tilde{\phi}(k)\equiv\int_{-\infty}^{+\infty}dx\,\phi(x)e^{-ikx}, \tag{4}$$

which exists for any normalizable, that is, square-integrable wave function of the system. The inverse Fourier transform is then defined as

$$\phi(x)\equiv\int_{-\infty}^{+\infty}\frac{dk}{2\pi}\tilde{\phi}(k)e^{ikx}. \tag{5}$$

It follows from Eq. (5) that

$$\phi''(x) = -\int_{-\infty}^{+\infty} \frac{dk}{2\pi} k^2 \tilde{\phi}(k) e^{ikx}, \tag{6}$$

and

$$x\phi'(x) = \int_{-\infty}^{+\infty} \frac{dk}{2\pi} k \tilde{\phi}(k) \frac{d}{dk}(e^{ikx})$$
$$= -\int_{-\infty}^{+\infty} \frac{dk}{2\pi} e^{ikx} \frac{d}{dk}[k\tilde{\phi}(k)]. \tag{7}$$

Equation (7) was obtained using integration by parts and assuming that $\tilde{\phi} \to 0$ as $k \to \infty$. By substituting Eqs. (5)–(7) into Eq. (3), I obtain after some minor algebra the first-order differential equation

$$2k \frac{d\tilde{\phi}}{dk} = -k^2 \tilde{\phi} + (2\epsilon - 1)\tilde{\phi}, \tag{8}$$

which can be integrated at once with the result

$$\tilde{\phi}(k) = Ck^{(2\epsilon-1)/2} e^{-k^2/4}. \tag{9}$$

Here C is an arbitrary constant. It readily follows from Eq. (9) that

$$\phi(x) = C\int_{-\infty}^{+\infty} dk\, k^{(2\epsilon-1)/2} e^{-k^2/4} e^{ikx}. \tag{10}$$

Hence, the formal solution for the eigenfunction of the harmonic oscillator is

$$\psi(x) = Ce^{x^2/2}\int_{-\infty}^{+\infty} dk\, k^{(2\epsilon-1)/2} e^{-k^2/4} e^{ikx}. \tag{11}$$

Recall that the eigenfunctions are either even or odd, that is,

$$\psi(-x) = \pm \psi(x). \tag{12}$$

It then follows from Eq. (11) that

$$\psi(-x) = Ce^{x^2/2}\int_{-\infty}^{+\infty} dk\, k^{(2\epsilon-1)/2} e^{-k^2/4} e^{-ikx}$$
$$= Ce^{x^2/2}\int_{-\infty}^{+\infty} dk(-k)^{(2\epsilon-1)/2} e^{-k^2/4} e^{ikx}, \tag{13}$$

where the right-hand side of Eq. (13) was obtained by making the change of variables $k \to -k$. It can be inferred from Eqs. (11) to (13) that the necessary and sufficient condition for the eigenfunctions to have a definite parity can be expressed as

$$(-1)^{(2\epsilon-1)/2} = \pm 1. \tag{14}$$

It follows that the allowed values of the energy ϵ_n must be quantized in terms of the nonnegative integer n, ($n = 0,1,2,3,\ldots$), that is,

$$\epsilon_n = n + 1/2. \tag{15}$$

It is seen from Eqs. (11) and (15) that negative values of n must be excluded because they do not lead to the normalizable eigenfunctions ψ_n. Equation (15) is the celebrated quantization condition for the energy levels of the harmonic oscillator.

By using Eq. (15), one can cast Eq. (11) into the form

$$\psi_n(x) = C_n e^{x^2/2}\int_{-\infty}^{+\infty} dk\, k^n e^{-k^2/4} e^{ikx}. \tag{16}$$

Equation (16) can be represented as

$$\psi_n(x) = C_n e^{x^2/2} \frac{d^n}{d(ix)^n} \int_{-\infty}^{+\infty} dk\, e^{-k^2/4} e^{ikx}. \tag{17}$$

The integral in Eq. (17) can be evaluated using the formula

$$\int_{-\infty}^{+\infty} dx\, e^{-x^2/4} e^{iax} = \sqrt{4\pi} e^{-a^2}. \tag{18}$$

On redefining the normalization constant C_n, I arrive at the result

$$\psi_n(x) = (-1)^n C_n e^{-x^2/2} e^{x^2} \frac{d^n}{dx^n} e^{-x^2}, \tag{19}$$

and finally,

$$\psi_n(x) = C_n e^{-x^2/2} H_n(x). \tag{20}$$

Here I have introduced the Hermite polynomials by the expression

$$H_n(x) \equiv (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}. \tag{21}$$

Equations (15), (20), and (21) represent a complete solution for the stationary states of a one-dimensional quantum harmonic oscillator.

In summary, I have presented an alternative method of finding the stationary states of a quantum mechanical harmonic oscillator which relies on the properties of Fourier transforms. The proposed approach makes it possible to determine the eigenfunctions of the oscillator with remarkable simplicity, and it provides valuable insight into the origin of the quantization condition for the energies of the eigenstates.

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[1]L. Schiff, *Quantum Mechanics* (McGraw–Hill, New York, 1968), 3rd ed.
[2]C. Cohen-Tannoudji, B. Diu, and F. Laloë, *Quantum Mechanics* (Wiley-Interscience, New York, 1977), Vol. I.
[3]A. Sommerfeld, *Wave Mechanics* (Academic, New York, 1929).
[4]In reality, of course, the ‘‘magical’’ termination of the series solution for half-integer values of the energy is directly related to the normalization condition for the wave functions. However, this connection often is obscure to the students because it involves rather complicated mathematics.
[5]J. J. Sakurai, *Modern Quantum Mechanics* (Addison–Wesley, Reading, MA, 1994).

Erratum: "What is a state in quantum mechanics?" [Am. J. Phys. 72 (3), 348–350 (2004)]

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In Eqs. (2), (3), (4), and (5) all the squares in the denominators should be replaced by first powers. Note also that some of the left-hand bars in expressions such as $|(\Psi, \Psi)|$ in these equations are missing. (All the vertical bars on these norms may of course be omitted.) The states Ψ_1 and Ψ_2 are assumed to be normalized.

I am indebted to Eric Chisolm for calling my attention to these errors.

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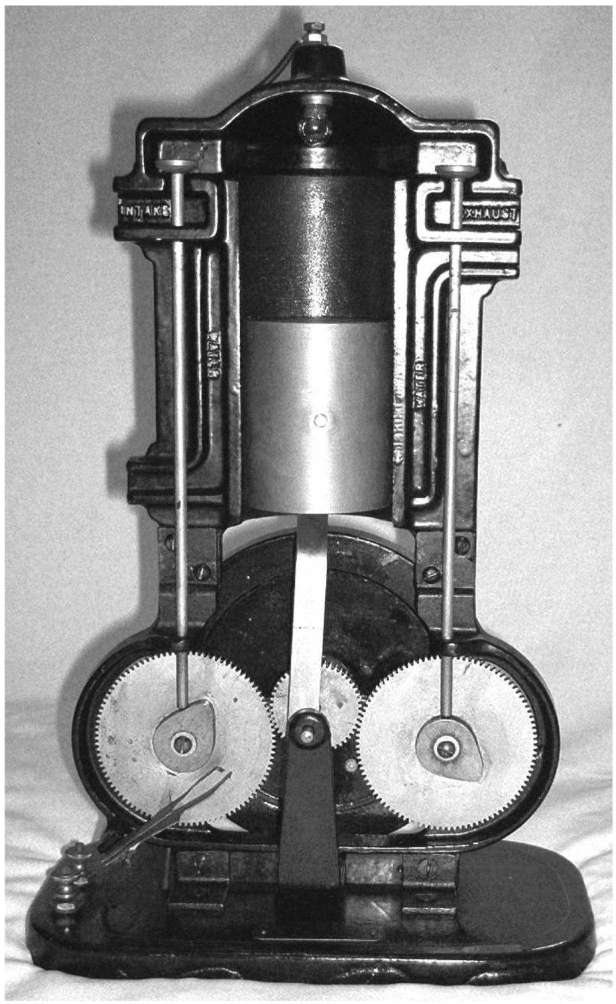

Gasoline Engine Half Model. This half model of a four-cycle gasoline engine was made by the Chicago Apparatus Co., and is listed at $25.00 in the 1936 catalogue. The large, heavy model is in the Greenslade collection and is 37.5 cm high. The words ''intake'' and ''exhaust'' are cast into the corresponding valve chambers, and the poppet valves themselves are operated by eccentrics cast into the two large gear wheels. The intake eccentric on the left also actuates a make-and-break contact that causes the light bulb at the top of the cylinder to flash, indicating the operation of the spark plug. On either side of the cylinder are chambers with the word ''water'' cast into them, indicating the jacket for cooling water. (Photograph and notes by Thomas B. Greenslade, Jr., Kenyon College)

