DS 8 & 9: One Dimensional Wave Mechanics

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Operators and their Representations

The Complex Plane

Let's work in a familiar space of complex numbers \mathbb{C} . Consider the position "vector" to an arbitrary point in this space, as shown in Figure (1). Suppose you now wish to *rotate* this vector by some angle φ to another point on the complex plane. It should be clear to you that we are would like to go from

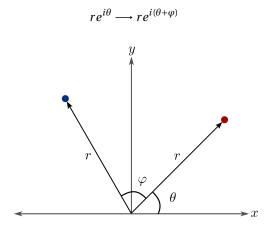


Figure 1: A rotation of a point on the complex plane by an angle φ .

Now, it should be clear that in this current "representation" of complex numbers (that is, as a real modulus times an imaginary exponential phase factor), this rotation is simply a multiplication by a phase factor $e^{i\varphi}$. i.e.

$$\mathbf{v}' = \hat{R}(\varphi)\mathbf{v} = e^{i\varphi} \cdot \mathbf{v}.$$

Now consider a *different* representation of complex numbers, namely the column vector representation. Since we can separate complex numbers into their real and imaginary parts (which are independent)

$$\mathbf{v} = \nu_x + i \, \nu_y,$$

we could be inspired by two-dimensional vectors and represent the same abstract v as a column-vector:

$$\underline{V} \equiv \begin{pmatrix} v_x \\ v_y \end{pmatrix}$$

Again, drawing from our study of 2D vector-spaces, it should be clear to you that we could represent a rotation by the appropriate matrix

$$\underline{\underline{R}}(\varphi) \equiv \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix},$$

such that the rotated vector V' is given by

$$\underline{V}' = \underline{\underline{R}}(\varphi) \cdot \underline{V} = \begin{pmatrix} \cos \varphi & -\sin \varphi \\ \sin \varphi & \cos \varphi \end{pmatrix} \cdot \begin{pmatrix} v_x \\ v_y \end{pmatrix}.$$

These two representations are obviously quite different, but they are both equivalent representations of complex numbers. Rotations of vectors in the complex plane can thus either be:

- (a) Multiplication by a pure phase $\hat{R}(\varphi)$ if we use the **v** representation: $\mathbf{v}' = \hat{R}(\varphi)\mathbf{v}$.
- (b) Multiplication by a matrix $\underline{R}(\varphi)$, if we use the \underline{V} representation: $\underline{V}' = \underline{R}(\varphi)\underline{V}$.

It should now be a straightforward thing to show that

$$\underline{V}' = \begin{pmatrix} v_x \cos \varphi - v_y \sin \varphi \\ v_x \sin \varphi + v_y \cos \varphi \end{pmatrix} \quad \text{and} \quad \mathbf{v}' = \left(v_x \cos \varphi - v_y \sin \varphi \right) + i \left(v_x \sin \varphi + v_y \cos \varphi \right)$$

represent the same complex number. All of this just goes to show that the abstract action of an operator (i.e. a "rotation") can be represented in different ways, depending on how we choose to represent our "vector".

3-Dimensional Space

Now let's consider a simple example you're already familiar with: 3D space. You know that vectors in 3D space can be represented in one of two ways:

$$\mathbf{v} = v_1 \hat{\mathbf{x}} + v_2 \hat{\mathbf{y}} + v_3 \hat{\mathbf{z}} \quad \text{or} \quad \underline{V} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}$$

Each of these representations has its own pros and cons. In particular, the first one makes it amply clear in *which* basis $(\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}})$ your vector is defined. However, in order to define the inner produce, you need to define new rules:

$$\hat{\mathbf{x}} \cdot \hat{\mathbf{x}} = 1$$
, $\hat{\mathbf{x}} \cdot \hat{\mathbf{y}} = 0$, $\hat{\mathbf{x}} \cdot \hat{\mathbf{z}} = 0$,

and so on, which you're familiar with.

On the other hand, the second representation does not need you to define new rules, the old rules of matrix multiplication are sufficient. However, it is not explicitly clear clear in *which* basis your vector is defined. Thus, a vector could be represented by a triplet

$$\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} v_1' \\ v_2' \\ v_3' \end{pmatrix}$$

depending on your choice of coordinate axes. Thus, when working with vectors as columns, *you need to be clear about your choice of basis*.

Finite Dimensional Hilbert Spaces

At the start of the course we dealt with two and three state quantum systems (like spin) where the state of the system $|\psi\rangle$ could be one of two (or three) possibilities. A simple example of this is indeed spin, where a particle's spin could be either $|\uparrow\rangle$ or $|\downarrow\rangle$. An arbitrary state can be expressed as a superposition of these states:

$$|\psi\rangle = \alpha |\uparrow\rangle + \beta |\downarrow\rangle$$

Such systems can be represented as a two-dimensional Hilbert space, and so we could choose to represent

$$|\uparrow\rangle$$
 by $\begin{pmatrix}1\\0\end{pmatrix}$ and $|\downarrow\rangle$ by $\begin{pmatrix}0\\1\end{pmatrix}$

Note: Why these particular linearly independent column vectors and no other? Since this is the **natural basis** of the problem. Consider a simple 2D space with two orthogonal vectors $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$. In the $\{\hat{\mathbf{x}}, \hat{\mathbf{y}}\}$ basis, the vector $\hat{\mathbf{x}}$ is just represented by $\hat{\mathbf{x}}$! If you had another basis, say $\{\hat{\mathbf{x}}', \hat{\mathbf{y}}'\}$, then the vector $\hat{\mathbf{x}}$ would be different (say $c_1\hat{\mathbf{x}}' + c_2\hat{\mathbf{y}}'$).

In such a basis, the vector $|\psi\rangle = \alpha |\uparrow\rangle + \beta |\downarrow\rangle$ can be represented by

$$|\psi\rangle$$
 is represented by $\Psi = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$

The components of the column are given by

"Top" component
$$=\langle \uparrow | \psi \rangle = \alpha$$
"Bottom" component $=\langle \downarrow | \psi \rangle = \beta$.

Operators in 2D Hilbert Spaces

Let's imagine we have an "operator" \hat{F} in this Hilbert space that "flips" spin. In other words, it makes a spin-up particle spin-down, and vice-versa. Thus

$$\hat{F} |\!\uparrow\rangle = |\!\downarrow\rangle$$

$$\hat{F} |\downarrow\rangle = |\uparrow\rangle$$

Note: Once the action of an operator is specified on all the basis vectors (as was done above) no more information is needed. Since any vector can be written as a linear sum of the basis vectors $\alpha \mid \uparrow \rangle + \beta \mid \downarrow \rangle$, the action of \hat{F} on such a vector can easily be calculated to be $\beta \mid \uparrow \rangle + \alpha \mid \downarrow \rangle$.

What about the column representation of vectors? How do operators act on them? Obviously, it is something that takes one column vector $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ to another $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$, and thus must be a 2 × 2 **matrix**. The components of this matrix are given by

$$F_{ij} = \langle i | \hat{F} | j \rangle$$
,

where $|i\rangle$, $|j\rangle$ could be either $|\uparrow\rangle$ or $|\downarrow\rangle$. Thus, calculating it explicitly,

$$F_{\uparrow\uparrow}=0$$
 $F_{\uparrow\downarrow}=1$

$$F_{\downarrow\uparrow} = 1$$
 $F_{\downarrow\downarrow} = 0$

We can reproduce the action of \hat{F} on an arbitrary state $\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$ through this matrix:

$$\underline{\underline{F}} \cdot \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \beta \\ \alpha \end{pmatrix}.$$

Going from abstract Dirac notation to Schrodinger's Wave Notation

Let's now try to apply these ideas to Quantum Mechanics. What we will be doing is simple: quantum systems are described by a **state**, a vector in an infinite dimensional Hilbert Space. However, it is much more convenient to work with a different representation: the **wavefunction** representation.

The idea behind this is the following: just as vectors may be represented as columns with each entry being the **component** of the vector in a certain "direction", we can do the same for $|\psi\rangle$. However, since the vector space is **infinite** dimensional, an infinite number of basis vectors are required. Three special bases will be quite important:

- (a) The energy basis, labelled as $|E\rangle$,
- (b) The position basis, labelled as $|x\rangle$, and
- (c) The momentum basis, labelled as $|p\rangle$

Any one of these bases can **completely** define the quantum state!¹ As a result, there is a one-to-one correspondence between the $|\psi\rangle$ and the "column vector" represented by (say) $\langle x|\psi\rangle$.

Discrete vs. continuous bases

Here we come to an important point: the position and momentum bases are special bases (unlike the spin basis in the previous example). Because of the structure of space and time, position is a **continuous basis**. The state $|x_0\rangle$ represents a particle **localised at** x_0 . As a result, x_0 may take any value from $-\infty$ to $+\infty$: an infinite number of possibilities. The same is true for the momentum basis $|p\rangle$. The energy basis $|E\rangle$ may be either discrete (as for bound states) or continuous (as for scattering states).

When we deal with such continuous bases, our "column vectors" become infinitely tall, and the spacing between the elements becomes infinitesimal: thus, we represent them by **functions**. The position space wavefunction (which is so commonly used that it's just called the "wavefunction") can be defined by

$$\Psi(x, t) = \langle x | \psi(t) \rangle$$

We could also define another function called the "momentum-space wavefunction", by taking the inner product with the set of momentum eigenstates:

$$\widetilde{\Psi}(p,t) = \langle p | \psi(t) \rangle$$

but we'll discuss this later. For this course, in general, it's a good idea to work in position space until you're sufficiently comfortable to be adventurous.

 $|\Psi(x,t)|^2 \iff$ Probability of finding the particle with position between x and x + dx $|\widetilde{\Psi}(p,t)|^2 \iff$ Probability of finding the particle with momentum between p and p + dp

The Schrodinger Equation

You should remember from the earlier classes that in the abstract "ket" representation the Schrodinger Equation can be written as:

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} |\psi\rangle = \hat{H} |\psi\rangle.$$

Th Hamiltonian \hat{H} is defined (as in Classical Mechanics) as

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}),$$

where position and momentum are **operators**. We can define these operators by their action on their basis states:

 $^{^{\}mathrm{1}}\mathrm{This}$ may be non-intuitive, so take some time to understand this.

$$\hat{x} | x_i \rangle = x_i | x_i \rangle$$

$$\hat{p} | p_i \rangle = p_i | p_i \rangle$$

where $|x_i\rangle$ (and $|p_i\rangle$) are the **states of definite position** (and states of definite momentum), and x_i (and p_i) their eigenvalues.

The Position Basis

Let us, from now on, work only in the position basis. In this basis, the action of the position operator is quite simple. Let us now ask the following question: if I have a state $|\psi\rangle$ which has an associated wavefunction $\Psi(x,t)$, what is the associated wavefunction for the state $\hat{x}|\psi\rangle$?

This is very easy to determine: we begin by expanding $|\psi\rangle$ in the position basis, and then take the \hat{x} operator into the integral:

$$\hat{x} | \psi \rangle = \hat{x} \Big(\int_{-\infty}^{\infty} |x'\rangle \langle x' | \psi \rangle \Big)$$
$$= \int_{-\infty}^{\infty} x' |x'\rangle \langle x' | \psi \rangle,$$

since $\hat{x} | x' \rangle = x' | x' \rangle$. To find the associated wavefunction to this state, we need to find $\langle x | \hat{x} | \psi \rangle$

$$\langle x | \hat{x} | \psi \rangle = \int_{-\infty}^{\infty} x' \langle x | x' \rangle \langle x' | \psi \rangle$$
$$= \int_{-\infty}^{\infty} x' \delta(x - x') \langle x' | \psi \rangle$$
$$= x \Psi(x, t)$$

where we have used the fact that the states $|x_i\rangle$ are orthonormal $(\langle x_i | x_j \rangle = \delta(x_i - x_j))$ and the defining property of the δ -function.

The action of the position operator on a state in the position basis is just to multiply the corresponding wavefunction by x. Thus, in the position basis,

$$\langle x | \hat{x} | \psi \rangle \longrightarrow \hat{x} \Psi(x, t) = x \Psi(x, t)$$

We could now do the same thing for the momentum operator. The proof is slightly involved, and I have given a similar proof in DS-5. You should go through your notes and show this:

The action of the momentum operator on a state in the position basis is:

$$\langle x | \hat{p} | \psi \rangle \longrightarrow \hat{p} \Psi(x, t) = \frac{\hbar}{i} \frac{\partial}{\partial x} \Psi(x, t).$$

Thus, to get the Schrodinger Equation in the **position** basis, all you need to do is replace:

$$\hat{x} \longrightarrow x$$

$$\hat{p} \longrightarrow \frac{\hbar}{i} \frac{\partial}{\partial x}$$

and act it on the wavefunction $\Psi(x, t)$. Thus,

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left|\psi\right\rangle = \left(\frac{\hat{p}^2}{2m} + V(\hat{x})\right)\left|\psi\right\rangle \Longleftrightarrow i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \left(\frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 + V(x)\right)\Psi(x,t)$$

This leads to the time-dependent Schrodinger Equation

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi$$

Solving the Equation

In **PHY201** we learnt how to solve Partial Differential Equations like the one above. The method was to *assume* that there exist solutions of the form $\psi(x)T(t)$, and plug it into the above equation. Rearranging the terms, this provides two *ordinary* differential equations which are always equal. The only way this is possible is if they are both equal to some constant (say, C). In our case:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V(x)\psi = C\psi$$
$$i\hbar\frac{\mathrm{d}T}{\mathrm{d}t} = CT$$

The first equation above is of the form: $\hat{H}\psi(x) = C\psi(x)$. This is unfortunately called the "time-independent Schrodinger Equation", but it's really better to call it the Energy-Eigenvalue equation. From the postulates of Quantum Mechanics we know that the Hamiltonian represents the energy of the system, and so $\psi_n(x)$ must be its eigenfunctions, and C should take the values of their respective energies E_n . We write down a subscript of P_n for each of the terms as there may be more than one function which satisfies the equation. As a result, we have

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi_n}{\mathrm{d}x^2} + V(x)\psi_n = E_n\psi$$
$$i\hbar\frac{\mathrm{d}T}{\mathrm{d}t} = E_nT$$

The solutions to the second equation are just $T(t) = N \exp\left\{-i\frac{E_n}{\hbar}t\right\}$. Thus, our separable solution is just

$$\psi(x)T(t) = N\psi_n(x)e^{-iEt/\hbar}$$
.

IMPORTANT: These are only the separable solutions, *NOT* the general solutions. These solutions are the **stationary** states of the system (i.e., the states of definite energy). However, a system may be in an arbitrary state, which will be a linear superposition of these states.

This is not unlike what happens on a string, where the "standing wave" solutions are sines and cosines, but you can construct any arbitrary wave (say, a Gaussian) on the string. Of course, the Gaussian **will not** be a *separable* solution of the wave equation, but it can be *constructed* from separable solutions.

The general solution to Schrodinger's Equation is given by

$$\Psi(x,t) = \sum_{n} c_n \psi_n(x) e^{-iE_n/\hbar}.$$

Notice that each term in the sum has its *own* (different!) phase factor. This leads us to a neat recipe to find $\Psi(x, t)$:

- (a) Find V(x).
- (b) Plug it into the energy-eigenvalue equation to find $\psi_n(x)$ and E_n .
- (c) The general solution is $\sum_{n} c_n \psi_n(x) e^{-iE_n t/\hbar}$.
- (d) To find c_n , use the initial conditions, and the fact that $\psi_n(x)$ are orthonormal.

Note: While this is very similar to the method to find the Fourier coefficients, it is not *exactly* the same. In the case of Fourier coefficients, the $\psi_n(x)$ functions were sines and cosines. In Quantum Mechanics, these functions are the stationary state functions of the quantum system: they *may* be sines and cosines (like in the Infinite Well), but they could be the Hermite Polynomials (the Harmonic Oscillator), the Bessel Functions (Infinite Cylindrical Well) and so on.

If the initial state is given to you as a linear combination of states of definite energy (or stationary states, or eigenstates of the Hamiltonian) then you do not have to calculate coefficients c_n , you can just read them off the linear superposition!

1 Problems

1.1 The Free Particle

Consider a free particle:

$$V(x) = 0$$
 (everywhere)

(a) Show that the two **separable** wavefunctions $\Psi(x, t)$ can be written as:

$$\Psi_1(x,t) = e^{-i\left(kx + \frac{E_1 t}{\hbar}\right)}$$

$$\Psi_2(x,t) = e^{+i\left(kx - \frac{E_2 t}{\hbar}\right)}$$

- (b) Find the energy eigenvalues E_1 and E_2 for each of these solutions. (Plug them into the energy-eigenvalue equation)
- (c) Show that the general solution can be written as

$$\Psi_k(x,t) = Ae^{+ik\left(x - \frac{\hbar k}{2m}t\right)} + Be^{-ik\left(x + \frac{\hbar k}{2m}t\right)}$$

Notice that the only difference in these two terms of the sum is the **sign** of *k*. Is this is state *also* a state of definite energy?

- (d) You've seen that $\Psi_1(x,t)$ and $\Psi_2(x,t)$ are states of definite energy. Are they also states of definite **momentum**? What about $\Psi_k(x,t)$?
- (e) Argue that the general solution to the Schrodinger Equation is

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{+ik\left(x - \frac{\hbar k}{2m}t\right)},$$

where A(k) are the Fourier coefficients of $\Psi(x, t)$. The overall factor of $\sqrt{2\pi}$ in the denominator is a sort of "normalisation" constant which comes from the definition of the Fourier transform.

Is this a state of definite momentum? Is this a state of definite energy?

1.2 Assorted 1D problems

- (a) Show that the commutator of two Hermitian operators is not Hermitian.
- (b) Show that for any 1D problem, the time-independent wavefunctions can be taken to be real.

Hint: In order to do this, first write the complex conjugate version of the energy-eigenvalue equation, and show that any linear combination of $\psi(x)$ and $\psi^*(x)$ satisfies the same equation.

(c) Show that the expectation value of momentum is always zero for any **real** wavefunction.

Hint: You can use the fact that The expectation values of physical observables must be real.

(d) Suppose the particle is prepared in a state $\phi(x)$ which is not real, so that $\langle \hat{p} \rangle_{\phi} = p$. Now consider the following state

$$\varphi(x)=\phi(x)e^{ip_0x/\hbar}.$$

Prove that $\langle \hat{p} \rangle_{\omega} = p + p_0$.

(e) Suppose at t=0, a free particle is prepared in a state of definite momentum $|\psi(0)\rangle = |p_0\rangle$. Show that

$$\Psi(x,t) = e^{i\lambda(t)}\Psi(x,0).$$

(f) Show that the Fourier Transform of a Gaussian is a Gaussian. Calculate the product of their standard deviations.

(g) Imagine a particle in state $|\psi\rangle$ described by a wavefunction

$$\psi(x) = \frac{N}{x^2 + a^2}$$

- (i) Calculate N.
- (ii) Calculate $\langle x \rangle$, Δx , $\langle p \rangle$, and Δp .
- (iii) Calculate $\widetilde{\psi}(p)$ and plot $|\widetilde{\psi}(p)|^2$.

1.3 Scattering Problems

(a) Consider a particle in approaching a **potential step**:

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & x > 0 \end{cases},$$

where $V_0 > 0$.

- (i) Let us first consider the case for $E < V_0$. Calculate the reflection coefficient.
- (ii) Now consider $E > V_0$. Calculate the reflection coefficient for this case.
- (iii) Calculate the transmission coefficient T for the case $E > V_0$. Show that it is **not** just the ratio of the transmitted (C) and incident (A) amplitudes. This is because the transmitted wave travels "slower". Show that

$$T = \sqrt{\frac{E - V_0}{E}} \frac{|C|^2}{|A|^2}.$$

1.4 The Particle in a Box

(a) You are given that a particle in an infinite well has stationary states given by

$$\psi_n(x) = \begin{cases} N \sin\left(\frac{n\pi x}{L}\right) & 0 \le x \le L \\ 0 & \text{otherwise.} \end{cases}$$

- (i) Calculate N.
- (ii) Plug this into the energy-eigenvalue equation and obtain the energy of the state n.
- (iii) Calculate the expectation value of the position $\langle x \rangle$ in an arbitrary state n.
- (iv) Calculate $\langle p \rangle$ in an arbitrary state n.
- (v) Show that $\int_{x_0}^{x_0 + \Delta x} |\psi_n(x)|^2 dx$ is independent of x_0 as $n \to \infty$. $(0 < x_0 < a, x_0 < a, x_0 + \Delta x < a)$

(b) Now suppose that the particle was *not* initially in a state of definite energy, but in some strange state, given by

$$\Psi(x,0) = \begin{cases} Nx(x-a), & 0 \le x \le a \\ 0, & \text{elsewhere.} \end{cases}$$

- (i) Calculate N.
- (ii) Find $\Psi(x, t)$. i.e. calculate the coefficients c_n in the sum

$$\Psi(x,t) = \sum_{n} c_n \psi_n(x) e^{-iE_n t/\hbar}.$$

- (iii) Find the ratios of the probabilities $P(E_n)/P(E_1)$ as a function of time.
- (iv) Find $\langle x \rangle$ and $\langle p \rangle$.
- (c) Consider the first problem given in Quiz 2, but relax the condition a little: suppose a particle in a box is prepared to be in a superposition of the first two states, with amplitudes $\cos \theta$ and $\sin \theta$ respectively.
 - (i) Find $\Psi(x,0)$.
 - (ii) Find $\Psi(x, t)$. Rewrite it using $\omega = \pi^2 \hbar / 2mL^2$.
 - (iii) Calculate $\langle x \rangle$, $\langle p \rangle$, σ_x , σ_p .
 - (iv) Does the time dependence for these quantities vanish for any values of θ ? If yes, which ones and why? If no, why not?
- (d) A particle is in a box of length a, prepared in a state

$$\Psi(x,0) = \begin{cases} N \sin(\frac{2\pi x}{a}) & 0 \le x \le a/2 \\ 0 & \text{otterwise} \end{cases}$$

- (i) Find *N*.
- (ii) Find $\Psi(x, t)$ and $|\Psi(x, t)|^2$. What is the most probable value of energy?
- (iii) Find $\langle x(t) \rangle$, $\langle p(t) \rangle$, $\langle E(t) \rangle$.

1.5 The Harmonic Oscillator

- (a) A particle of mass m starts off in the ground state of the harmonic oscillator. Find $\langle x(t) \rangle$ for this state.
- (b) A particle of mass m in the harmonic oscillator potential starts out with the state

$$\Psi(x,0) = A \left(1 - 2\sqrt{\frac{m\omega}{\hbar}}x\right)^2 e^{-\frac{m\omega}{2\hbar}x^2}$$

(i) What is $\langle E \rangle$?

(ii) At some late time T, the wavefunction is

$$\Psi(x,T) = B \left(1 + 2\sqrt{\frac{m\omega}{\hbar}} x \right)^2 e^{-\frac{m\omega}{2\hbar} x^2}$$

for some constant B. What is the smallest possible value of T?