T-Reflection in Quantum Mechanics

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Personal Section

My first real physics course in my freshman year of high school sparked within me an interest in the field that burned on as I then studied physics topics on my own, participated in physics competitions, and took more advanced classes in my junior year. I had always enjoyed the elegance and purity of math, so I was drawn to those same elements in physics. Thus, when I was choosing a field in which I would complete a research project in the summer before my senior year, physics was a natural choice. I was drawn to the strange world of quantum theory and fundamental physics, so I sought out Dr. Thomas Cohen in the Department of Physics at the University of Maryland, College Park to mentor and guide me in a project in that area of physics. When Dr. Cohen suggested that I do work involving a recently proposed and little-understood property in physics called T-reflection, and told me about the potential importance of T-reflection to understanding dark energy, a great mystery to physics, I was intrigued by the prospect of working with something so new and potentially powerful.

Since theoretical physics is often mathematically intensive, I naturally spent quite a bit of time working with math in the course of my work. As I had never studied quantum mechanics before, I had to familiarize myself with the basics before I could start work. In order to get comprehend some of the concepts of quantum mechanics, I also had to l some learn linear algebra beyond what I had seen in school. When it came to my task for the project, which involved completing a pair of proofs concerning T-reflection in a quantum mechanical system called the harmonic oscillator, I had to perform substantial algebraic manipulation, connect in calculus topics that I had learned in school, and apply proof techniques that I had developed from participation in the school math team, while also picking up instrumental new mathematical knowledge from the undergraduate student who I worked with in addition to Dr. Cohen, Nathan Borak, in order to succeed.

My summer research experience taught me some important lessons about what it takes to work on and succeed in a research project. The power of persistence has no equal, a truth that I picked up as I had to put in two weeks of hard thought to complete each proof. In addition, team work, as well as never being afraid to seek help when needed, are indispensable, which I learned when I had to frequently ask the people around me for help with understanding new quantum mechanical concepts and for suggestions when I got stuck in the course of formulating the proofs. Therefore, to an aspiring researcher, I would suggest never giving up and never being afraid to ask questions as two important ideas to remember in the course of work.

All in all, I found research to be an exciting way to see the power of math in action as a strong backbone for scientific discovery while learning cool new mathematical and scientific knowledge, as well as important life lessons for how to work on substantial projects. It was a rewarding experience of immeasurable value.

Research Section

Introduction

One of the great remaining mysteries of modern physics is the accelerating expansion of the universe. It has been proposed that dark energy is responsible for this phenomenon. In order to understand dark energy, it is necessary to compute the energy density of the vacuum that arises from the fundamental field theories that describe the universe. The vacuum energy density appears in Einstein's theory of general relativity as the famous cosmological constant, and was first introduced in order to establish a static universe [1]. General relativity would have otherwise predicted an expanding or contracting universe, and it was generally believed at the time that the universe was not changing in size. Later, when Hubble discovered that the universe was indeed expanding, Einstein discarded the constant [1]. However, there is nothing in general relativity that forbids the introduction of the cosmological constant [1], and today, it is clear that its value must be found if one is to use general relativity to explain dark energy.

It is assumed that the vacuum energy density arises from the vacuum energies of the quantum field theories (QFTs) describing the fundamental forces (these energies are also known as the zero point or ground state energies) [2]. If one were able to develop a single QFT describing the fundamental forces of our universe, determining the zero point energy of that theory would allow determination of the cosmological constant. Unfortunately, the vacuum energy in a QFT is rather ill-posed. In particular, if one neglects gravitational effects, only energy differences, rather than absolute energies, have experimental consequences [2]. Consequently, there is no empirical way to determine the natural zero point energy of a QFT.

Recently, a property called T-reflection has been proposed [3] that may provide a handle for determining the zero point energies for quantum systems, including QFTs. T-reflection has already proved to be a useful tool in the study of various field theories [4, 5]. While it is far from certain that the theory underlying our universe would necessarily possess well-defined behavior under T-reflection, it is still useful to examine T-reflection, as it is one of the very few known tools in physics that would allow one to set a natural zero point energy for a QFT.

If a function describing a physical quantity is said to have well-defined behavior under T-reflection, it means that the modulus of the quantity is invariant under the reflection of the temperature $T \to -T$. This is to say that, for some quantity $f(\beta)$ dependent on $\beta = \frac{1}{k_b T}$, $f(\beta) = e^{i\theta} f(-\beta)$. Of course, the notion of examining negative temperature might seem to be completely nonsensical. After all, in systems where the energy is bounded below, but not above, temperature only has physical sense when T is on the interval $[0, \infty)$. However, T-reflection is not truly an investigation of negative temperature. Rather, it is an examination of the mathematical function describing the physical quantity when that function is continued to negative β. Thus, negative T is being used in a purely mathematical, as opposed to physical, sense. There are two types of well-defined T-reflection behavior of note. A quantity is said to be odd under T-reflection if $f(\beta) = -f(-\beta)$, and is said to be even if $f(\beta) = f(-\beta)$.

First, a critical property of T-reflection will be discussed. This is that changing the ground state energy of a quantum mechanical system eliminates any previous well-defined behavior under T-reflection symmetry [3]. This property can be illustrated with a simple example, the partition function of the harmonic oscillator. The partition function is an important quantity in statistical mechanics, and is defined as $Z(\beta) := \sum_n e^{-\beta E_n}$, where n are the microstates of the system, and E_n is the energy in state n [7]. The harmonic oscillator has energy given by $E_n = \hbar\omega(n + \frac{1}{2})$, so the harmonic oscillator partition function is given by $Z(\beta) = \frac{1}{2\sinh\frac{\beta\hbar\omega}{2}}$. This partition function, as noted in [3], has well-defined behavior under T-reflection. Note that if the ground state energy $\frac{1}{2}\hbar\omega$ is shifted by some quantity Δ, the energy would become $E_n = \hbar\omega(n + \frac{1}{2}) + \Delta$ and the partition function would become $Z(\beta) = \frac{e^{-\beta\Delta}}{2\sinh\frac{\beta\hbar\omega}{2}}$. This partition function does not possesses well-defined behavior under T-reflection. In general, changing the ground state energy by non-zero Δ multiplies the partition function by a factor of $e^{-\beta\Delta}$, which would always eliminate any previous well-defined behavior under T-reflection. This means that having well-defined behavior under T-reflection essentially fixes the ground state energy to some value [3]. This property is precisely why T-reflection could be useful for the cosmological constant problem. If the theory underlying our universe has well-defined behavior under T-reflection, only one value for the zero point energy for the theory would allow the preservation of the well-defined behavior.

It has been previously noted that well-defined behavior under T-reflection is present in the partition functions of numerous quantum field theories in addition to the quantum harmonic oscillator [3]. Having a partition function with well-defined behavior under T-reflection says that the thermal expectation values of certain observables will have well-defined behavior under T-reflection as well. This is because the partition function $Z(\beta)$ can be used to directly derive the expectation values of various thermodynamic quantities, such as, for example, powers of the thermodynamic energy, which can be written as $\langle \hat{E}^k \rangle_T = (-1)^k \frac{1}{Z}\frac{\partial^k Z}{\partial \beta^k}$, where k is a non-negative integer [7]. By various identities concerning derivatives and products of even and odd function, $\langle E^k \rangle$ has well-defined behavior under T-reflection for all k if Z has well-defined behavior under T-reflection: it is even for even k, and it is odd for odd k. In fact, it is clear that as long as some expectation value can be written as the product of Z and its derivatives, and the partition function has well-defined behavior under T-reflection, the expectation value will have well-defined behavior under T-reflection as well.

Given the potential importance of T-reflection in fundamental physics, it is important to develop intuition and insight about its properties. While previous papers have only examined T-reflection in partition functions [3], this paper shows for the first time that a wide class of observables not directly derived from the partition function exhibit well-defined behavior under T-reflection. For the sake of simplicity, this paper will examine the harmonic oscillator, which, as noted above, has a partition function with well-defined behavior under T-reflection. The behavior of the thermal expectation value of $\langle \hat{x}^k \rangle_T$, where k is an non-negative integer, under T-reflection will be determined in section 2 by deriving and examining an explicit expression for $\langle \hat{x}^k \rangle_T$. Generalization to the behavior of a larger class of Hermitian combinations of $\hat{x}$ and $\hat{p}$ under T-reflection will be discussed. Finally, the conclusions made in the course of this paper will be summarized. Many of the mathematical derivations that support the results of this paper are somewhat but involved. For the sake of readability and brevity, these are relegated to the appendices.

T-Reflection and Powers of $\hat{x}$

The thermal expectation value of $\hat{x}^k$ in the harmonic oscillator, where k is a non-negative integer, will now be calculated and examined for well-defined behavior under T-reflection. The cases where $\langle \hat{x}^k \rangle_T = 0$ need not be considered, as $\langle \hat{x}^k \rangle_T$ is already well behaved in that case. Thus, the case of odd k is unimportant. An argument for why the thermal expectation vanishes in this case is given in Appendix A. It is possible to derive the expression

$$\langle \hat{x}^k \rangle_T = (\frac{\hbar}{m\omega})^{\frac{k}{2}} \frac{k!}{2^k \frac{k}{2}!} \coth^{\frac{k}{2}} \frac{\beta\hbar\omega}{2} \tag{1}$$

for even k.

A more detailed description of the derivation of (1) is included in Appendix A, but a brief outline of the proof will be given here. Since only even k matter, k will be written as $2b$, where b is a non-negative integer. First, an expression for $\langle n|\hat{x}^{2b}|n\rangle$ is derived (the result is (5) in Appendix A). It is shown to be equal to $(\frac{\hbar}{m\omega})^b \frac{(2b)!}{2^{2b} b!} \frac{\frac{d^n}{dy^n} \frac{(1+y)^b}{(1-y)^{b+1}}|_{y=0}}{n!}$. The latter expression is a multiple of the coefficient of the nth term of the Maclaurin series of $\frac{(1+y)^b}{(1-y)^{b+1}}$, which can be found in (6) in Appendix A. This equality allows one to find an expression for $\sum_{n=0}^{\infty} \langle n|\hat{x}^{2b}|n\rangle \, e^{-\beta\hbar\omega n}$, which is (10) in Appendix A. This expression is then substituted into the definition of $\langle \hat{x}^k \rangle_T$ to yield (1).

The significance of the expression found for $\langle \hat{x}^k \rangle_T$ is that when T is taken to $-T$, $\langle \hat{x}^k \rangle_T = (-1)^{\frac{k}{2}} \langle \hat{x}^k \rangle_{-T}$ for even k, since $\coth(x) = -\coth(-x)$. This means that the parity of $\langle \hat{x}^k \rangle_T$ under T-reflection goes with the parity of $\frac{k}{2}$. Thus, the quantity $\langle \hat{x}^k \rangle_T$ has well-defined behavior under T-reflection for non-negative integral k. This is a powerful result, as it is the first time that the thermal expectation of an observable not directly derivable from the partition function has been shown to have well-defined behavior under T-reflection.

However, not all observables are guaranteed to have well-defined behavior under T-reflection. For instance, the class of observables $\langle \hat{x}^k + \hat{x}^{k+2} \rangle_T$, where k is a non-negative even integer, does not have well-defined behavior under T-reflection, as $\langle \hat{x}^k \rangle_T$ and $\langle \hat{x}^{k+2} \rangle_T$ have opposite parity under T-reflection, and the sum of two quantities that have different parities has no parity.

T-Reflection and More Generalized Hermitian Operators of $\hat{x}$ and $\hat{p}$

The T-reflection properties of the thermal expectation value of Hermitian sums of products of $\hat{x}$ and $\hat{p}$ (operators such as $\hat{x}^2\hat{p}^4\hat{x}^2$ or $\hat{x}\hat{p}^2\hat{x}^3 + \hat{x}^3\hat{p}^2\hat{x}$) are now examined. In particular, it is shown that the thermal expectation of a Hermitian operator that is a sum of products of $\hat{x}$ and $\hat{p}$, where each term has j factors of $\hat{x}$ and k factors of $\hat{p}$ (for example, $\hat{x}\hat{p}^2\hat{x}^3 + \hat{x}^3\hat{p}^2\hat{x}^3$ is such an expression, where $j = 4$ and $k = 2$) have the parity of $\frac{j+k}{2}$ under T-reflection if j and k are even, and the parity of $\frac{j+k}{2} - 1$ if j and k are odd. The thermal expectation vanishes when j and k are of different parity, so that case is disregarded; this is true by an argument based on parity.

Demonstrating this claim first requires examining the behavior of $\langle \hat{x}^j\hat{p}^k + \hat{p}^k\hat{x}^j \rangle_T$ and $\langle i(\hat{x}^j\hat{p}^k - \hat{p}^k\hat{x}^j) \rangle_T$ under T-reflection. It is shown that the parity of $\langle \hat{x}^j\hat{p}^k + \hat{p}^k\hat{x}^j \rangle_T$ goes with that of $\frac{j+k}{2}$ when j and k are even, and that the parity of $\langle i(\hat{x}^j\hat{p}^k - \hat{p}^k\hat{x}^j) \rangle_T$ goes with that of $\frac{j+k}{2} - 1$ when j and k are odd. As shown in Appendix B, $\langle \hat{x}^j\hat{p}^k + \hat{p}^k\hat{x}^j \rangle_T$ vanishes when either j or k is odd, and $\langle i(\hat{x}^j\hat{p}^k - \hat{p}^k\hat{x}^j) \rangle_T$ vanishes when either j or k is even, so those cases also are not examined. The behavior of $\langle \hat{x}^j\hat{p}^k + \hat{p}^k\hat{x}^j \rangle_T$ and $\langle i(\hat{x}^j\hat{p}^k - \hat{p}^k\hat{x}^j) \rangle_T$ under T-reflection for j and k such that the thermal expectations do not vanish can be summarized in the following set of equations:

$$\begin{aligned} \langle \hat{x}^j\hat{p}^k + \hat{p}^k\hat{x}^j \rangle_T &= (-1)^{\frac{j+k}{2}} \langle \hat{x}^j\hat{p}^k + \hat{p}^k\hat{x}^j \rangle_{-T} \qquad && j,k \text{ even} \\ \langle i(\hat{x}^j\hat{p}^k - \hat{p}^k\hat{x}^j) \rangle_T &= (-1)^{\frac{j+k}{2}-1} \langle i(\hat{x}^j\hat{p}^k - \hat{p}^k\hat{x}^j) \rangle_{-T} && j,k \text{ odd} \end{aligned} \tag{2}$$

A more detailed explanation of the derivation for (2) is given in Appendix B, but a brief outline is given here. It is shown that the behavior of $\langle \hat{x}^j\hat{p}^k + \hat{p}^k\hat{x}^j \rangle_T$ is equivalent to that of $\langle \hat{x}^j\hat{p}^k \rangle_T$ under T-reflection for even j and k, and that the behavior of $\langle i(\hat{x}^j\hat{p}^k - \hat{p}^k\hat{x}^j) \rangle_T$ is equivalent to that of $\langle \hat{x}^j\hat{p}^k \rangle_T$ under T-reflection for odd j and k. Thus, even though $\hat{x}^j\hat{p}^k$ is not a Hermitian operator, the proof is greatly simplified if one examines the behavior of $\langle \hat{x}^j\hat{p}^k \rangle_T$ under T-reflection. A recursive expression for $\langle \hat{x}^j\hat{p}^k \rangle_T$ is derived using the Hamiltonian operator and commutators, resulting in (14) in Appendix B. This expression is then used to prove that the parity of $\langle \hat{x}^j\hat{p}^k \rangle_T$ under T-reflection goes with the parity of $\frac{j+k}{2}$ when j and k are even, and that it goes with the parity of $\frac{j+k}{2} - 1$ when j and k are odd using induction, completing the derivation.

Any Hermitian sum of products of $\hat{x}$ and $\hat{p}$ where each term has j factors of $\hat{x}$ and k factors of $\hat{p}$ can be written as a linear combination of $\langle \hat{x}^j\hat{p}^k + \hat{p}^k\hat{x}^j \rangle_T$ and $\langle i(\hat{x}^j\hat{p}^k - \hat{p}^k\hat{x}^j) \rangle_T$ terms. This shall be called the "standard form." The veracity of this statement can be seen if one notes that if Hermitian operator $\hat{A}$ is written as $\sum_n \hat{B}_n$ for some $\hat{B}_n$, then $\hat{A} = \sum_n \frac{\hat{B}_n + \hat{B}_n^\dagger}{2}$, and sees that the original Hermitian sum of products of $\hat{x}$ and $\hat{p}$ can be written as a linear combination of $\hat{x}^j \hat{p}^k$ terms using the commutator $[\hat{x}, \hat{p}]$, where terms with even j and k have real coefficients and those with odd j and k have imaginary coefficients. Also, commuting an $\hat{x}$ and a $\hat{p}$ in an expression with j factors of $\hat{x}$ and factors of k $\hat{p}$ yields a term with j factors of $\hat{x}$ and k factors of $\hat{p}$ plus a term with $j-1$ factors of $\hat{x}$ and $k-1$ factors $\hat{p}$. Therefore, by (2), all the terms in the standard form of a Hermitian sum of products of $\hat{x}$ and $\hat{p}$ where each term has j factors of $\hat{x}$ and k factors of $\hat{p}$ have the same parity under T-reflection, and that parity goes with that of $\frac{j+k}{2}$ if j and k are even, and with that of $\frac{j+k}{2} - 1$ if j and k are odd. Since all the terms in the standard form follow this parity rule, the original Hermitian combination also does, completing the derivation of the claim at the beginning of this section.

This is a powerful result, as it shows that the thermal expectations of a large class of observables in a quantum mechanical system have well-defined behavior under T-reflection.

Conclusion

This paper first showed that the thermal expectation values of a specific class of observables, $\hat{x}^k$, have well-defined behavior under T-reflection. This result was then used to show the behavior of a class Hermitian sums of products of the position and momentum operators under T-reflection. This is the first time that the thermal expectation values of observables not directly derivable from the partition function have been shown to have well-defined behavior under T-reflection. At the same time, it was also shown that not all observables will necessarily have well-defined behavior under T-reflection. In sum, the work in this paper provides a new insight on T-reflection: that some, but not all, observables independent of the partition function exhibit well-defined behavior under T-reflection. Since T-reflection has the potential to help solve the dark energy problem and improve understanding of the dynamics of the universe, greater knowledge of T-reflection is a possibly critical part of solving one of the most important remaining problems in modern physics.

Appendix A: Derivation of $\langle \hat{x}^k \rangle_T$

It will now be shown that

$$\langle \hat{x}^k \rangle_T = (\frac{\hbar}{m\omega})^{\frac{k}{2}} \frac{k!}{2^k \frac{k}{2}!} \coth^{\frac{k}{2}} \frac{\beta \hbar \omega}{2} \tag{3}$$

for even k. Only the case of even k matters, as will later be explained in this section.

For the sake of simplicity, units where $\hbar = m = \omega = 1$ will be used throughout this discussion. Since a dimensionless quantity cannot be made out of the three constants, there is a unique way to reinsert them in a dimensionally correct manner. It is thus is possible to reinsert the constants later using dimensional analysis.

The derivation is greatly simplified with the introduction of the notation ?, which generalizes the standard notion of the factorial. It shall be defined that if $a > b$, $\frac{a?}{b?} := a(a-1)...(b+1)$ and that if $a < b$, $\frac{a?}{b?} := \frac{1}{b(b-1)...(a+1)}$, and that if $a = b$, $\frac{a?}{b?} := 1$. Also, it is defined that $0? := 1$. This definition of the ? operation is essentially a way to ensure that a ratio of factorials is always well-defined for integers.

The following will also be defined: $\binom{n}{k}_? := \frac{n?}{k?}\frac{0?}{(n-k)?} = \frac{n?}{(n-k)?}\frac{0?}{k?}$. This definition effectively acts as a continuation of $\binom{n}{k}$ for all integral n and k.

The definition of the thermal expectation value of $\hat{x}^k$ can be simplified to

$$\langle \hat{x}^k \rangle_T = (1 - e^{-\beta}) \sum_{n=0}^{\infty} \langle n|\hat{x}^k|n\rangle \, e^{-\beta n} \tag{4}$$

in the case of the harmonic oscillator.

$\langle n|\hat{x}^k|n\rangle = 0$ when k is odd, so from (4) $\langle \hat{x}^k \rangle_T$ also vanishes for odd k. As the behavior under T-reflection is already well-defined in that case, this justifies why the rest of this discussion will examine only the case of even $k = 2b$, where b is a non-negative integer.

It can be shown that

$$\langle n|\hat{x}^{2b}|n\rangle = \frac{(2b)?}{2^{2b} b?} \sum_{i=0}^{b} (-1)^i \binom{b}{i}_? \binom{n+2b-2i}{2b}_? \tag{5}$$

using the expression of the expectation value in integral form, properties of the Hermite polynomials, and differentiation under the integral.

To proceed with the derivation, it is useful to have an expression for the nth coefficient of the Maclaurin series for the function $f(y) = \frac{(1+y)^b}{(1-y)^{b+1}}$, which is found to be

$$\frac{\frac{d^n}{dy^n} \frac{(1+y)^b}{(1-y)^{b+1}} |_{y=0}}{n?} = \sum_{i=0}^{n} \binom{n}{i}_? \binom{b+i}{n}_? \tag{6}$$

using Leibniz'general product rule.

It can also be shown that

$$\langle n|\hat{x}^{2b}|n\rangle = \frac{(2b)?}{2^{2b}b?}\frac{\frac{d^n}{dy^n}\frac{(1+y)^b}{(1-y)^{b+1}}|_{y=0}}{n?} \tag{7}$$

after demonstrating that

$$\langle n|\hat{x}^{2b}|n\rangle = \frac{(2b)?}{2^{2b}b?}\frac{\frac{d^b}{dy^b}\frac{(1+y)^n}{(1-y)^{n+1}}|_{y=0}}{b?} \tag{8}$$

using induction and showing that

$$\frac{\frac{d^n}{dy^n}\frac{(1+y)^b}{(1-y)^{b+1}}|_{y=0}}{n?} = \frac{\frac{d^b}{dy^b}\frac{(1+y)^n}{(1-y)^{n+1}}|_{y=0}}{b?} \tag{9}$$

using some algebraic manipulation and (6).

Using (7) in conjunction with setting $y = e^{-\beta}$ in the Maclaurin series for $f(y) = \frac{(1+y)^b}{(1-y)^{b+1}}$, it can be seen that

$$\sum_{n=0}^{\infty}\langle n|\hat{x}^{2b}|n\rangle\, e^{-\beta n} = \frac{(2b)!}{2^{2b}b!}\frac{(1+e^{-\beta})^b}{(1-e^{-\beta})^{b+1}} \tag{10}$$

Plugging this into (4) gives

$$\langle\hat{x}^{2b}\rangle_T = \frac{(2b)!}{2^{2b}b!}(\frac{1+e^{-\beta}}{1-e^{-\beta}})^b = \frac{(2b)!}{2^{2b}b!}\coth^b\frac{\beta}{2}$$

Reinserting $\hbar$, m, and ω, and replacing b with $\frac{k}{2}$ gives (3). QED

Appendix B: Behavior of $\langle\hat{x}^j\hat{p}^k + \hat{p}^k\hat{x}^j\rangle_T$ and $\langle i(\hat{x}^j\hat{p}^k - \hat{p}^k\hat{x}^j)\rangle_T$ Under T-Reflection

It is shown that the parity of $\langle\hat{x}^j\hat{p}^k + \hat{p}^k\hat{x}^j\rangle_T$ goes with that of $\frac{j+k}{2}$ when j and k are even, and that the parity of $\langle i(\hat{x}^j\hat{p}^k - \hat{p}^k\hat{x}^j)\rangle_T$ goes with that of $\frac{j+k}{2} - 1$ when j and k are odd. This is to say that

$$\langle\hat{x}^j\hat{p}^k + \hat{p}^k\hat{x}^j\rangle_T = (-1)^{\frac{j+k}{2}}\langle\hat{x}^j\hat{p}^k + \hat{p}^k\hat{x}^j\rangle_{-T} \tag{11}$$

for even j and k and

$$\langle i(\hat{x}^j\hat{p}^k - \hat{p}^k\hat{x}^j)\rangle_T = (-1)^{\frac{j+k}{2}-1}\langle i(\hat{x}^j\hat{p}^k - \hat{p}^k\hat{x}^j)\rangle_{-T} \tag{12}$$

for odd j and k.

The case of even j and k is the only significant one for $\langle\hat{x}^j\hat{p}^k + \hat{p}^k\hat{x}^j\rangle_T$, and only the case of odd j and k is significant for $\langle i(\hat{x}^j\hat{p}^k - \hat{p}^k\hat{x}^j)\rangle_T$, as will be explained later in this section.

For the sake of simplicity, units where $\hbar = m = \omega = 1$ will be used throughout this discussion.

Although $\hat{x}^j\hat{p}^k$ is not a Hermitian operator, examining its properties under T-reflection will be useful for showing the behavior under T-reflection of $\langle \hat{x}^j\hat{p}^k + \hat{p}^k\hat{x}^j\rangle_T$ and $\langle i(\hat{x}^j\hat{p}^k - \hat{p}^k\hat{x}^j)\rangle_T$ for reasons that will be explained in this subsection.

First, the thermal expectation value of $\hat{x}^j\hat{p}^k$ is in the case of the harmonic oscillator

$$\langle \hat{x}^j\hat{p}^k\rangle_T = (1 - e^{-\beta}) \sum_{n=0}^{\infty} \langle n|\hat{x}^j\hat{p}^k|n\rangle\, e^{-\beta n} \tag{13}$$

Also, if one writes $\langle n|\hat{x}^j\hat{p}^k|n\rangle$ as an integral, it can be seen that the integrand is odd when j and k are of different parity, the integral vanishes when j and k do not have the same parity.

It can also be derived that $\langle \hat{x}^j\hat{p}^k\rangle_T = (-1)^k\, \langle \hat{p}^k\hat{x}^j\rangle_T$.

Therefore, $\langle \hat{x}^j\hat{p}^k + \hat{p}^k\hat{x}^j\rangle_T$ vanishes when either j or k is odd, and $\langle i(\hat{x}^j\hat{p}^k - \hat{p}^k\hat{x}^j)\rangle_T$ vanishes when either j or k is even. The cases where the thermal expectation vanishes are insignificant as behavior under T-reflection is well-defined in that case, and so will not be considered.

It is also clear that the parity of $\langle \hat{x}^j\hat{p}^k + \hat{p}^j\hat{x}^k\rangle_T$ and of $\langle i(\hat{x}^j\hat{p}^k - \hat{p}^k\hat{x}^j)\rangle_T$ will be the same as that of $\langle \hat{x}^j\hat{p}^k\rangle_T$ when $\langle \hat{x}^j\hat{p}^k + \hat{p}^j\hat{x}^k\rangle_T$ and $\langle i(\hat{x}^j\hat{p}^k - \hat{p}^k\hat{x}^j)\rangle_T$ do not vanish. Thus, it suffices to examine the behavior of $\langle \hat{x}^j\hat{p}^k\rangle_T$ under T-reflection if one wishes to know the behavior of $\langle \hat{x}^j\hat{p}^k + \hat{p}^k\hat{x}^j\rangle_T$ and $\langle i(\hat{x}^j\hat{p}^k - \hat{p}^k\hat{x}^j)\rangle_T$ under T-reflection.

In order to show the behavior of $\langle \hat{x}^j\hat{p}^k\rangle_T$ under T-reflection, it is first useful to derive a recursive expression for $\langle \hat{x}^j\hat{p}^k\rangle_T$ when $k \geq 2$. The following expression can be found using the Hamiltonian and the commutator $[\hat{p}^n, \hat{x}^2]$.

$$\begin{aligned}\langle \hat{x}^j\hat{p}^k\rangle_T = &-2\frac{\partial}{\partial\beta}\langle \hat{x}^j\hat{p}^{k-2}\rangle_T + \coth\frac{\beta}{2}\,\langle \hat{x}^j\hat{p}^{k-2}\rangle_T - \langle \hat{x}^{j+2}\hat{p}^{k-2}\rangle_T \\ &+ \begin{cases} 0 & k=2 \\ 2i\,\langle \hat{x}^{j+1}\rangle_T & k=3 \\ 2i(k-2)\,\langle \hat{x}^{j+1}\hat{p}^{k-3}\rangle_T + (k-2)(k-3)\,\langle \hat{x}^j\hat{x}^{k-4}\rangle_T & k\geq 4 \end{cases}\end{aligned} \tag{14}$$

The following statement can then be proved with use of the recursive expression above, the results derived in Appendix A, and strong induction.

$$\langle \hat{x}^j\hat{p}^k\rangle_T = \begin{cases} (-1)^{\frac{j+k}{2}}\,\langle \hat{x}^j\hat{p}^k\rangle_{-T} & j,k \text{ even} \\ (-1)^{\frac{j+k}{2}-1}\,\langle \hat{x}^j\hat{p}^k\rangle_{-T} & j,k \text{ odd} \end{cases} \tag{15}$$

Another way to state this is to say that the parity of $\langle \hat{x}^j \hat{p}^k \rangle_T$ under T-reflection is the parity of $\frac{j+k}{2}$ if j and k are even, and that it is the parity of $\frac{j+k}{2} - 1$ if j and k are odd.

As noted earlier, the parity of $\langle \hat{x}^j \hat{p}^k + \hat{p}^k \hat{x}^j \rangle_T$ and $\langle \hat{x}^j \hat{p}^k \rangle_T$ under T-reflection is the same when the expressions do not vanish, so (11) follows from (15). Similarly, since the parity of $\langle i(\hat{x}^j \hat{p}^k - \hat{p}^k \hat{x}^j) \rangle_T$ under T-reflection goes with that of $\langle \hat{x}^j \hat{p}^k \rangle_T$ when the expressions do not vanish, (12) also follows from (15). QED

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