PROBLEM SET 6

DUE DATE: Thursday, April 3, 2008, at 5:00 p.m. in the 8.323 homework box, at the intersection of the 3rd floor of building 8 and the 4th floor of building 16.

REFERENCES: Lecture Notes #5: Path Integrals for One-particle Quantum Mechanics, on the website. Peskin and Schroeder, Secs. 9.1-9.3.

Problem 1: Proof of \( e^A e^B = e^{A+B+\frac{1}{2}[A,B]} \) (10 points)

In discussing particle creation by a classical source, we made use of the identity

\[ e^A e^B = e^{A+B+\frac{1}{2}[A,B]} , \]  

which is true whenever \( A \) and \( B \) are operators which both commute with \([A,B]\): 

\[ [A, [A,B]] = 0 , \quad [B, [A,B]] = 0 . \]  

This identity is a special case of the Baker-Campbell-Hausdorff identity, which does not require condition (1.2), and for which the exponent on the right-hand side of Eq. (1.1) is an infinite series of iterated commutators beginning with the terms shown here. Your assignment for this problem is to prove Eq. (1.1), using Eqs. (1.2).

**Suggestion:** One way to do it is to introduce a parameter \( \lambda \), to allow the operators to be varied continuously from zero to their full values. That is, one can write Eq. (1.1) for the operators \( \lambda A \) and \( \lambda B \):

\[ e^{\lambda A} e^{\lambda B} = e^{\lambda A + \lambda B + \frac{1}{2} \lambda^2 [A,B]} . \]  

If one defines 

\[ F_1(\lambda) \equiv e^{\lambda A} e^{\lambda B} , \]  

\[ F_2(\lambda) \equiv e^{\lambda A + \lambda B + \frac{1}{2} \lambda^2 [A,B]} , \]  

then our goal is to prove that \( F_1(\lambda) = F_2(\lambda) \). Clearly 

\[ F_1(0) = F_2(0) = I , \]  

where \( I \) is the identity operator, and 

\[ \frac{dF_1(\lambda)}{d\lambda} = (A + B) F_1(\lambda) . \]  

The problem is then solved if we can show that \( F_2(\lambda) \) also satisfies the differential equation (1.6), since the differential equation and the initial condition (1.5) determine the solution uniquely.
Problem 2: A Composite Operator (15 points)

Since $\phi(x)$ is not an operator, but instead an operator-valued distribution, the quantity $\phi^2(x)$ is not defined. There is no general definition for the square of a distribution. For example, you are probably aware that the square of a delta-function makes no sense. Nonetheless it is possible to define a composite operator $\phi^2(x)$: which has some, but not all, of the properties that one would naively expect for the square of the operator $\phi(x)$. Note for example that some operator of this sort is necessary to give a quantum treatment to the energy density, which classically is given by

$$T^{00} = \frac{1}{2} \dot{\phi}^2 + \frac{1}{2} \nabla \phi \cdot \nabla \phi + \frac{1}{2} m^2 \phi^2 . \quad (2.1)$$

The other terms lead to similar issues in their definition, but for now we will deal only with the $\phi^2$ term. The other terms can be treated in the same way, so by the time you finish this problem you will be prepared to calculate the quantum properties of $T^{00}$.

Starting with

$$\phi(x) = \int \frac{d^3p}{(2\pi)^3} \frac{1}{\sqrt{2E_p}} \{ a(\vec{p}) e^{-i\vec{p}\cdot\vec{x}} + a^\dagger(\vec{p}) e^{i\vec{p}\cdot\vec{x}} \} , \quad (2.2)$$

it seems natural to define

$$\phi^2(x) : \equiv \int \frac{d^3p}{(2\pi)^3} \frac{1}{\sqrt{2E_p}} \int \frac{d^3q}{(2\pi)^3} \frac{1}{\sqrt{2E_q}} \left\{ a(\vec{p}) a(\vec{q}) e^{-i(\vec{p}+\vec{q})\cdot\vec{x}} \right\} \quad (2.3)$$

The above expression is obtained by naively squaring the expression in Eq. (2.2), and then normal ordering, which means to move the annihilation operators to the right of the creation operators. (To combine the two cross-terms one must also realize that $\vec{p}$ and $\vec{q}$ are variables of integration, so their names can be interchanged.) Since the commutator of a creation and annihilation operator is a c-number, the normal ordering is equivalent to subtracting a c-number from the expression. The c-number can be viewed as the vacuum expectation value of the expression before normal ordering. The c-number subtraction is infinite, since the commutator is integrated over $\vec{p}$.

The $:\ $ notation indicates normal ordering, which is essential in defining a $\phi^2$ operator that gives finite matrix elements for physical states. To make sense out of Eq. (2.3), however, one must remember that it must not be considered an operator, but rather an operator-valued distribution. Eq. (2.3) is correct, but its interpretation has some subtleties to explore.
(a) Show that
\[ \langle 0 \mid :\phi^2(x) : :\phi^2(y) : \mid 0 \rangle = 2D^2(x - y), \] (2.4)
where
\[ D(x - y) \equiv \langle 0 \mid \phi(x) \phi(y) \mid 0 \rangle. \] (2.5)
This is a special case of Wick’s theorem, which we will learn about in Chapter 4 of Peskin and Schroeder.

(b) Since \( :\phi^2(x) : \) is an operator-valued distribution, let us integrate it with a smooth weight function to see if we obtain a well-behaved operator. Call the weight function \( w(\vec{x}) \), and consider the quantity
\[ O_3[w] \equiv \int d^3 x w(\vec{x}) :\phi^2(\vec{x}, t) :. \] (2.6)
The normal ordering insures that \( \langle 0 \mid O_3[w] \mid 0 \rangle = 0 \), so the vacuum variance of \( O_3[w] \) is given by
\[ \sigma^2 = \langle 0 \mid O^2_3[w] \mid 0 \rangle = \int d^3 x d^3 y w(\vec{x}) w(\vec{y}) \langle 0 \mid :\phi^2(\vec{x}, t) : :\phi^2(\vec{y}, t) : \mid 0 \rangle \]
\[ = 2 \int d^3 x d^3 y w(\vec{x}) w(\vec{y}) D^2(\vec{x} - \vec{y}). \] (2.7)
For spacelike separations we know from Problem Set 4 that
\[ D(x - y) = \frac{m}{4\pi^2 r} K_1(m r), \] (2.8)
where \( K_1(z) \) denotes a modified Bessel function, as defined for example in Gradshteyn and Ryzhik (Table of Integrals Series and Products, Academic Press), and \( r^2 = -(x - y)^2 \). Use the asymptotic behavior of the modified Bessel function to show that the integral in Eq. (2.7) does NOT converge.

To cure the convergence problem, two steps are necessary. First, to regulate \( :\phi^2(x) : \) we must smear in time as well as in space. This is the generic case in quantum field theories—the field \( \phi(x) \) represents the unusual case in which smearing in space alone is sufficient. So we introduce a smearing function \( w(x^\mu) \) for 4-vectors, and define
\[ O_4[w] \equiv \int d^4 x w(x^\mu) :\phi^2(x^\mu) :. \] (2.9)
The analogue to Eq. (2.7) is then
\[ \sigma^2 = \langle 0 \mid O^2_4[w] \mid 0 \rangle = \int d^4 x d^4 y w(x^\mu) w(y^\mu) \langle 0 \mid :\phi^2(x^\mu) : :\phi^2(y^\mu) : \mid 0 \rangle \]
\[ = 2 \int d^4 x d^4 y w(x^\mu) w(y^\mu) D^2(x^\mu - y^\mu). \] (2.10)
This step alone does not quite solve the problem, because the integral will still have a divergence when $x^\mu$ is very near $y^\mu$. The right answer is finite, however, and the ambiguity of the integration shown in (2.10) can be eliminated in several alternative ways.

The ambiguity arises because $\langle 0 | :\phi^2(x^\mu) : :\phi^2(y^\mu) : | 0 \rangle$ was treated in Eq. (2.10) as if it were an ordinary function, while in fact it must be considered a distribution. To understand its definition as a distribution, we can go back to Eq. (2.9). The right-hand side cannot be interpreted as an ordinary integral, because $:\phi^2(x^\mu) :$ is not a function. When we say that $:\phi^2(x^\mu) :$ is a distribution, we mean that it is a recipe for defining an operator for every acceptable test function $w(x^\mu)$. Eq. (2.9) does not define $O_4[w]$ as an integral, but is instead just a symbolic way of saying the $O_4[w]$ is the result of applying the distribution $:\phi^2(x^\mu) :$ to the test function $w(x^\mu)$. The explicit definition of $O_4[w]$ can be obtained by using Eq. (2.3) to replace $:\phi^2(x) :$ on the right-hand side of Eq. (2.9). One can then integrate over $x^\mu$, giving an expression of the form

$$O_4[w] = \int \frac{d^3p}{(2\pi)^3} \frac{1}{\sqrt{2p^0}} \int \frac{d^3q}{(2\pi)^3} \frac{1}{\sqrt{2q^0}} \left\{ a(\vec{p}) a(\vec{q}) \tilde{w}(-q^\mu - p^\mu) + \ldots \right\}, \quad (2.11)$$

where

$$\tilde{w}(p^\mu) \equiv \int d^4x \ w(x^\mu) e^{i\vec{p} \cdot \vec{x}} \quad (2.12)$$

is the Fourier transform of $w(x^\mu)$, and $p^0$ and $q^0$ on the right-hand side are determined by the usual relations $p^0 = \sqrt{\vec{p}^2 + m^2}$, $q^0 = \sqrt{\vec{q}^2 + m^2}$. Note that integrating over $x^\mu$ before integrating over $\vec{p}$ and $\vec{q}$ appears to be a change in the order of integration, and such changes are often unjustified when divergent integrals are involved. However, our goal is to define the distribution $:\phi^2(x^\mu) :$, which is synonymous with defining $O_4[w]$. Eq. (2.11) is the definition we need, and Eq. (2.3) is correct only in the sense that it is interpreted as shorthand for Eq. (2.11).

(c) Fill in the “...” part of Eq. (2.11).

(d) Use your expression for Eq. (2.11) to express $\langle 0 | O_4^2[w] | 0 \rangle$ as a convergent integral over two three-vectors $\vec{p}$ and $\vec{q}$, treating $w(x^\mu)$ as an arbitrary test function.

Pedagogical Note: Another way to get the right answer is to use Eq. (2.10), but with an appropriate definition for $D(x^\mu - y^\mu)$ as a distribution. This is the approach normally followed for the Feynman propagator (i.e., the time-ordered product), Eq. (2.59) of Peskin and Schroeder:

$$D_F(x - y) \equiv \int \frac{d^4p}{(2\pi)^4} \frac{i}{p^2 - m^2 + i\epsilon} e^{-ip \cdot (x-y)} . \quad (2.13)$$
As we will see later, amplitudes are calculated by inserting the Feynman propagator into integrals which are always carried out before the limit $\epsilon \to 0$ is taken. This is one way of defining a distribution. The analogous expression for the simple (non-time-ordered) product is a refinement of Peskin and Schroeder’s Eq. (2.50):

$$D(x - y) = \langle 0 | \phi(x) \phi(y) | 0 \rangle = \int \frac{d^3p}{(2\pi)^3} \frac{1}{2E_p} e^{-ip \cdot (x-y-\i\epsilon n)} = \int \frac{d^4p}{(2\pi)^3} \delta(p^2 - m^2) \theta(p^0) e^{-ip \cdot (x-y-\i\epsilon n)},$$

(2.14)

where $n^\mu = (1, 0, 0, 0)$ is a unit vector in the positive time direction. Note that the insertion of the $i\epsilon$ term causes the integral to be absolutely convergent, and it also regularizes the infinity that would otherwise occur for $x = y$. With the $i\epsilon$ in place the integral in Eq. (2.10) becomes absolutely convergent, which allows the integrations to be rearranged to match the answer that you should have found in part (d).

(e) Consider the special case where $w(x^\mu)$ is a normalized Gaussian in both space and time:

$$w(x^\mu) = \frac{1}{\pi^{3/2}a^3} e^{-|\vec{x}|^2/a^2} \cdot \frac{1}{\sqrt{\pi}b} e^{-(x^0)^2/b^2}. \tag{2.15}$$

For fixed $b$, show that

$$\langle 0 | O_4[w] | 0 \rangle \xrightarrow{a \to \infty} \text{const} a^\beta, \tag{2.16}$$

where $\beta$ is a constant that you are to determine. (You need not find the constant of proportionality.) Does $\beta$ agree with what you found in Problem Set 3, Problem 1, for the variance of a smeared scalar field $\phi(x^\mu)$? Does this agree with what we would expect from the assumption that in the limit of large $a$, $O_4[w]$ samples many independent values of $\phi^2$?

(f) One property that one might naively expect for the square of an operator is positivity, but $\phi^2(x^\mu)$ is not positive. (Heuristically we can imagine that we constructed $\phi^2$ by first squaring $\phi$, but then we made an infinite subtraction which spoils the positivity.) Show that $\phi^2$ is not positive by constructing a state $|\psi\rangle$ such that

$$\langle \psi | O_4[w] | \psi \rangle < 0, \tag{2.17}$$

using the Gaussian weight function of Eq. (2.15). I would recommend looking for a state $|\psi\rangle$ of the form

$$|\psi\rangle = |0\rangle + \delta |\psi_1\rangle, \tag{2.18}$$

where $\delta$ is an arbitrarily small positive constant, so that only contributions to first order in $\delta$ need be considered. You need not evaluate $\langle \psi | O_4[w] | \psi \rangle$ completely, as long as you show that it is negative.
Problem 3: Application of path integrals: The harmonic oscillator in thermal equilibrium (15 points)

The study of a harmonic oscillator in thermal equilibrium provides a beautiful illustration of how path integrals can save work. Consider a harmonic oscillator described by the Hamiltonian

\[ H = \frac{1}{2}(p^2 + \omega^2 q^2) , \]  

where I have chosen units for which the mass \( m \) is unity. The canonical commutation relations, as usual, imply that

\[ [q, p] = i , \]  

where \( \hbar \) has also been set equal to one. Creation and annihilation operators can be defined by

\[ a^\dagger = \frac{1}{\sqrt{2\omega}}(p + i\omega q) \]
\[ a = \frac{1}{\sqrt{2\omega}}(p - i\omega q) . \]  

(a) Show that the canonical commutation relations (3.2) imply that

\[ [a, a^\dagger] = 1 . \]  

(b) Using the creation and annihilation operators, show that the energy \( E_n \) of the \( n \)th excited state is given by

\[ E_n = \left( n + \frac{1}{2} \right) \omega , \]  

and that

\[ \langle n | q^2 | n \rangle = \frac{1}{\omega} \left( n + \frac{1}{2} \right) . \]  

(c) To find the expectation value of \( q^2 \) in the canonical ensemble with temperature \( T \), canonical methods are very effective. The canonical ensemble expression for \( \langle q^2 \rangle \) is given by

\[ \langle q^2 \rangle = \frac{1}{Z} \sum_{n=0}^{\infty} e^{-\beta E_n} \langle n | q^2 | n \rangle , \]  

where

\[ \beta = \frac{1}{kT} , \]
$k$ is Boltzmann’s constant, and

$$Z = \sum_{n=0}^{\infty} e^{-\beta E_n}. \quad (3.9)$$

Show that

$$Z = \frac{1}{2 \sinh \left( \frac{1}{2} \beta \omega \right)}, \quad (3.10)$$

and find an expression for $\langle q^2 \rangle$ in terms of $\beta$ and $\omega$.

(d) While canonical methods allow one to find $\langle q^2 \rangle$ fairly easily, it is much harder to find the probability distribution for measurements of the coordinate $q$. The probability density $P(\bar{q})$ is defined so that the probability of finding $q$ between $\bar{q}$ and $\bar{q} + dq$ is given by $P(\bar{q}) dq$. For the eigenstate $|n\rangle$, $P(\bar{q}) = |\psi_n(\bar{q})|^2$, where $\psi_n(\bar{q})$ is the Schrödinger wave function. In the thermal ensemble, the probability density is given by

$$P(\bar{q}) = \frac{1}{Z} \sum_{n=0}^{\infty} e^{-\beta E_n} |\psi_n(\bar{q})|^2. \quad (3.11)$$

This sum is rather difficult to evaluate using canonical methods, but can be evaluated relatively easily by using path integral methods. Begin by showing that Eq. (3.11) can be rewritten as

$$P(\bar{q}) = \frac{1}{Z} \langle \bar{q} | e^{-\beta H} | \bar{q} \rangle. \quad (3.12)$$

Eq. (3.12) can be evaluated as a path integral, thinking of it as describing evolution by “imaginary time” $-i\beta$. The path integral expression is given by

$$\langle \bar{q} | e^{-\beta H} | \bar{q} \rangle \propto \int_{\tau=-\beta/2}^{\tau=\beta/2} Dq(\tau) \left| e^{-SE[q(\tau)]} \right|, \quad (3.13)$$

where

$$SE[q(\tau)] = \frac{1}{2} \int_{-\beta/2}^{\beta/2} d\tau \left\{ \left( \frac{dq}{d\tau} \right)^2 + \omega^2 q^2 \right\}. \quad (3.14)$$

is the Euclideanized action, where “Euclideanized” means that it has been analytically continued to imaginary time. The derivation of this path integral expression is completely analogous to the derivation given in class for the “real time” case, and you are not asked to repeat it.
(e) The path integral (3.13) can be evaluated by finding a classical solution which extremizes the Euclidean action, and then shifting variables to use new variables that describe the deviation from this classical solution. As a first step, find the classical solution \( q_{cl}(\tau) \) which extremizes the action (3.14), and satisfies the required boundary conditions: \( q_{cl}(-\beta/2) = q_{cl}(\beta/2) = \bar{q} \).

(f) Keeping in mind that in the path integral \( q(\tau) \) describes an infinite set of integration variables, one for each \( \tau \), define a new set of integration variables

\[
q'(\tau) = q(\tau) - q_{cl}(\tau).
\]

Show that

\[
S_E[q(\tau)] = S_E[q'(\tau)] + S_E[q_{cl}(\tau)].
\]

That is, show that cross terms involving both \( q'(\tau) \) and \( q_{cl}(\tau) \) vanish.

(g) Use these results to show that

\[
P(\bar{q}) = \frac{1}{\sqrt{2\pi} \sigma} e^{-q^2/(2\sigma^2)},
\]

where

\[
\sigma^2 = \frac{1}{2\omega} \coth \left( \frac{1}{2} \beta \omega \right).
\]

Remember that once one has used the path integral to determine the answer up to an unknown constant of proportionality, that constant can be fixed by normalizing the probability distribution so that it integrates to one. Is your result consistent with the expectation value that you found in part (c)?

[NOTE: For more information about path integrals, see for example Feynman and Hibbs, *Quantum Mechanics and Path Integrals* (McGraw Hill, 1965). Problems of this sort are discussed in Chapter 10.]