Quantum Canonical Transformations revisited

A.Y. Shiekh
International Centre for Theoretical Physics, Miramare, Trieste, Italy

Abstract
A preferred form for the path integral discretization is suggested that allows the implementation of canonical transformations in quantum theory.

1 Canonical Transformations in Quantum Theory

Canonical transformations are of great utility in classical theory [Goldstein, 1980]; however they do not work so well in quantum theory, giving rise to anomalous (order $\hbar^2$) potential like terms [Gervais and Jevicki, 1980; Klauder, 1980]. Despite the age of the problem of quantum canonical transformations, it continues to inspire interest [Anderson, 1993; 1993; 1994; 1994; Swanson, 1994].

Although equally applicable to quantum field theory, there is no virtue in working within its added complexity, and the problem is discussed in the context of quantum mechanics. This issue is well investigated in the setting of the Hamiltonian (phase space) path integral formulation of quantum theory [Feynman, 1948; 1965; Fanelli, 1976], due to its closeness to classical theory with its commuting variables. A transition amplitude is then generally written as:

$$\langle q_b, t_b | q_a, t_a \rangle = \int_{-\infty}^{\infty} Dq \int_{-\infty}^{\infty} Dp \frac{e^{i \bar{h} \int p \dot{q} - H(q, p, t) dt}}{2\pi \bar{h}}$$

which is formal because it actually depends upon how it is discretized. In general, each integral of the discretized path integral has a leading error of order $\Delta t$, and this error is not lost in the limit of infinite time refinement because there are $T\Delta t$ integrals ($T \equiv t_b - t_a$). So this error makes a finite contribution in the final limit, and it is exactly in this sensitivity to $\Delta t$ that the discretization scheme and equivalently the operator ordering of the operator formalism expresses itself [Schulman, 1981; Mayes and Dowker, 1972; 1973]. However, if one could locate a scheme with error of higher order than $\Delta t$, no contribution would be hidden, and one might anticipate a better behaved object under formal manipulations. The idea is that in moving into this scheme from another, the hidden error would be exposed and correctly accommodated within the proposed canonical transformation.

For an investigation of the error, end point integrations can be neglected, since the abandonment of any finite number of $\Delta t$ corrections will make no difference to the total error in the small time limit. Advantage will be taken of this simplification throughout.

Although there will be a formal investigation, it might be productive to first embark upon some numerical experiments to show the existence of the types of objects sought.
2 A ‘numerical’ Investigation

In the normal scheme, the standard path integral discretization is given by a variety of non-equivalent forms, a typical example with end points \((q_a, p_a), (q_b, p_b)\) being:

\[
I_\infty = \lim_{N \to \infty} \left\{ \int_{-\infty}^{+\infty} \cdots \int_{-\infty}^{+\infty} \prod_{j=1}^{N-1} dq_j \prod_{i=1}^{N} dp_i \exp \left( \frac{i}{\hbar} \sum_{k=1}^{N} (p_k(q_k - q_{k-1}) - H(q_{k-1}, p_k)\Delta t) \right) \right\}
\]

where \(\Delta t = \frac{T}{N}\)

It is well known, and will be confirmed below (both numerically and analytically), that each of the above integrals has an error of order \(\Delta t\). But just as the definition of the normal derivative has various forms of differing error (of relevance to computer numerics), namely:

\[
\frac{dx}{dt} \equiv \lim_{\Delta t \to 0} \frac{x(t + \Delta t) - x(t)}{\Delta t}
\]

or

\[
\frac{dx}{dt} \equiv \lim_{\Delta t \to 0} \frac{x(t + \Delta t) - x(t - \Delta t)}{2\Delta t}
\]

the first being accurate to order \(\Delta t\), and the second to order \((\Delta t)^2\); so one might also seek a path integral scheme with higher order error. There is a candidate in the more symmetric (mid-point) form given by [Shiekh, 1988; Klauder, 1980; Daubechies and Klauder, 1985]:

\[
\bar{I}_\infty = \lim_{M \to \infty} \int_{-\infty}^{+\infty} \cdots \int_{-\infty}^{+\infty} \prod_{j=1}^{2M} dq_j \prod_{i=0}^{2M+1} dp_i \exp \left( \frac{i}{4\hbar} \sum_{k=1}^{2M} \left( p_{k+1} - q_{k+1} - q_k \right) - H(q_k, p_k, t_k)\Delta t \right)
\]

where \(\Delta t = \frac{T}{2M+1}\)

This symmetric discretization for the path integral exists only for even subdivisions, and the first three time subdivision refinements are listed in the appendix, where Wick rotation \((t \to -it)\) has been performed to improve numerical convergence, having set \(\hbar = 1\) and dropped the end integrations, an act which does not effect the error contribution in the small time limit, but simplifies matters.

The traditional form (equation [3]) is known to have an error of order \(\Delta t\), while the symmetric form might be anticipated to have a higher order error. This might first be investigated numerically before proceeding analytically, with all end points held to zero (a coherent state like path integral).

These integrals differ from the limit by \(\int = \int_\infty^{+\infty} + \alpha(\Delta t)^n + \ldots\), so (adopting the notation where the subscript on \(I\) indicates the number of \(q\) (or \(p\) integrations):

\[
\int_2 = \int_\infty^{+\infty} + \alpha \left( \frac{1}{3}T \right)^n + \ldots
\]

\[
\int_4 = \int_\infty^{+\infty} + \alpha \left( \frac{1}{5}T \right)^n + \ldots
\]

\[
\int_6 = \int_\infty^{+\infty} + \alpha \left( \frac{1}{7}T \right)^n + \ldots
\]
Eliminating $\int_\infty$ and $\alpha$ in order to isolate the leading order error yields:

$$\frac{\int_6 - \int_4}{\int_4 - \int_2} = \frac{7^n - 5^n}{5^n - 3^n}$$

(9)

For a leading order error of $(\Delta t)^1$ one would get a ratio of $\frac{3}{7}$ for small evolution times, while for $(\Delta t)^2$ one would get a value of $\frac{27}{98}$. Using the trial Hamiltonian of a simple harmonic oscillator, namely:

$$H = \frac{1}{2} (p^2 + q^2)$$

(10)

avoids the heavy numerical work involved in the accurate evaluation of a twelve dimensional integration (in fact, the integrals were performed analytically with a computer mathematics package). Using a short evolution time of $T = 0.1$, and fixing the end points at zero, leads to the result for the normal path integral:

$$\frac{I_6 - I_4}{I_4 - I_2} = \frac{.9978625573 \ldots - .9980047869 \ldots}{.9980047869 \ldots - .998368743 \ldots} = .42829 \ldots$$

(11)

the $\frac{3}{7}$ ($0.42857 \ldots$) confirming that the leading order error is indeed $(\Delta t)^1$; while for the symmetric form one gets:

$$\frac{T_6 - T_4}{T_4 - T_2} = \frac{.9951226146 \ldots - .9952203945 \ldots}{.9952203945 \ldots - .9955752212 \ldots} = .27557 \ldots$$

(12)

the $\frac{27}{98}$ ($0.27551 \ldots$) corresponding to a leading order error of $(\Delta t)^2$, so confirming the suspicion that a higher order scheme will be free of hidden contributions.

3 Stochastic Terms

The chance is taken here to derive the well-known results that in the path integral $p \sim (\Delta t)^{-\frac{1}{2}}$ and $\Delta q \sim (\Delta t)^{\frac{1}{2}}$. An important exception to this rule is derived below.

Beginning from the Hamiltonian path integral, which consists of many integrals of the form:

$$\int dq \int dp \exp \left( \frac{i}{\hbar} \left( p \Delta q - H(q, p, t) \Delta t \right) \right)$$

(13)

It is assumed here that one is not dealing with unphysical, higher derivative theories (which would demand higher order 'momenta') so that the momentum is not found higher than quadratic order or negative powers. As a result the canonical transformation is somewhat limited in that it should not map to a theory of higher order, and the integral becomes:

$$\int dq \int dp \exp \left( \frac{i}{\hbar} \left( p \Delta q - \left( \frac{p^2}{2m(q, t)} + \gamma(q, t) p + V(q, t) \right) \Delta t \right) \right)$$

(14)

The $p$ integral may then be performed using the Gaussian result:
\[
\int_{-\infty}^{\infty} e^{-\alpha s^2 - \beta s} ds = \sqrt{\frac{\pi}{\alpha}} e^{\frac{\beta^2}{4\alpha}}
\]  

(15)

Now since the \( p^2 \) generates a \( 1/\alpha \), where \( \alpha = i\Delta t/2m\hbar \), so each \( p \) (for even powers) contributes like \((\Delta t)^{-\frac{1}{2}}\), while \( p \) alone generates a \( \beta^2 \), i.e. \(-\gamma (\Delta q - \Delta\Delta t)^2/\hbar^2\), so that \( p \) in odd powers contributes like \((\Delta t)^{\frac{1}{2}}\). In performing the \( p \) integrals in equation (14) and so obtaining the Lagrange formalism; \( p \) becomes \( m(\Delta q \Delta t - \gamma) \), so each \( p \) (for even powers) contributes like \((\Delta t)^{-\frac{1}{2}}\), while \( p \) alone generates a \( \beta^2 \), i.e. \(-\gamma (\Delta q - \Delta\Delta t)^2/\hbar^2\), so that \( p \) in odd powers contributes like \((\Delta t)^{\frac{1}{2}}\). This higher order contribution for odd powers will be crucial later.

It is in this way that the contributing class of paths are seen to be stochastic (or Brownian) in nature. This behaviour of the path integral must be carefully accounted for when working to order \( \Delta t \).

4 Canonical Transformations in the Symmetric Path Integral

In classical mechanics a canonical transformation is one that preserves the least action principle [Goldstein, 1980]. For the path integral one might analogously require that there be a path integral representation in the new variables \((Q, P, t)\), if one existed in the old ones \((q, p, t)\). The fact that the symmetric path integral has no ‘hidden’ parts should guarantee that formal canonical transformations are now valid. This in explicitly demonstrated below.

A canonical transformation should be system independent, that is to say, the transformation should be canonical not only for some specific system, but for all problems with the same degrees of freedom. The amplitude may alter under such a transformation by at most a phase factor. So \textit{formally} one gets:

\[
\exp \left( \frac{i}{\hbar} \int_{t_a}^{t_b} (p\dot{q} - H(q, p, t)) dt \right)
\]

(16)

with \( F(q, Q, t) \) being an arbitrary smooth function. Since the above equation is to be true for all Hamiltonians, one gets:

\[ p\dot{q} - H = P\dot{Q} - K + \frac{dF}{dt} \]  

(17)

the same condition as in classical mechanics, with \( F \) the generating function of the canonical transformation. For \( F = F(q, Q, t) \) one gets:

\[ p\dot{q} - H = P\dot{Q} - K + \frac{\partial F}{\partial q} \bigg|_{Q,t} \dot{q} + \frac{\partial F}{\partial Q} \bigg|_{q,t} \dot{Q} + \frac{\partial F}{\partial t} \bigg|_{q,Q} \]  

(18)

from which follows, by the independence of \( q \) and \( Q \):

\[ p = \frac{\partial F}{\partial q} \bigg|_{Q,t} \]  

(19)
\[ P = -\frac{\partial F}{\partial Q} \bigg|_{q,t} \]  
\[ K = H + \frac{\partial F}{\partial t} \bigg|_{q,Q} \]

All this work was formal, and now one is ready to apply this machinery to the symmetric discretization of the path integral in the hope that there will be no corrections. The formal canonical transformation of equation 16 now becomes (ignoring end integrals):

\[
\lim_{M \to \infty} \int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} \prod_{j=1}^{2M} dq_j \prod_{i=1}^{2M} dp_i \frac{1}{4\pi \hbar} \exp \left( \frac{i}{\hbar} \sum_{k=1}^{2M} \frac{p_k q_{k+1} - q_{k-1}}{2} - H(q_k, p_k, t_k) \Delta t \right)
\Rightarrow \lim_{M \to \infty} \int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} \prod_{j=1}^{2M} dQ_j \prod_{i=1}^{2M} dP_i \frac{1}{4\pi \hbar} \exp \left( \frac{i}{\hbar} \sum_{k=1}^{2M} \frac{P_k Q_{k+1} - Q_{k-1}}{2} - K(Q_k, P_k, t_k) \Delta t + \Delta F \right)
\]

where: \( \Delta F \equiv \frac{F(q_{k+1}, Q_{k+1}, t_{k+1}) - F(q_{k-1}, Q_{k-1}, t_{k-1})}{2} \)

Now, \( F \) itself, like all other terms in the action, cannot be worse than \((\Delta t)^0\) in strength, for the same reason given before that ‘higher derivative’ actions are excluded from this discussion. By expanding \( F \) and also using the facts that \( \Delta q \sim (\Delta t)^{1/2} \) and \( \Delta Q \sim (\Delta t)^{1/2} \) for even powers, and \( \sim (\Delta t)^1 \) for odd powers, one gets the crucial result:

\[
\Delta F = \frac{\partial F}{\partial Q} \bigg|_{q,t} \Delta Q + \frac{\partial F}{\partial q} \bigg|_{Q,t} \Delta q + \frac{\partial F}{\partial t} \bigg|_{q,Q} \Delta t + O(\Delta t)^{3/2}
\]

Had one not used the symmetric scheme, anomalous \((\hbar^2)\) terms would have entered here with the even powers of \( \Delta q \) and \( \Delta Q \) then present\(^1\). Dropping the \((\Delta t)^{3/2}\) term in the above (it is a \( \Delta t \) term that does not disappear in the limit) leads to:

\[
\Delta F = -P \Delta Q + p \Delta q + \frac{\partial F}{\partial t} \bigg|_{q,Q} \Delta t
\]

and from this one gets the anomaly free transformation of \( p \Delta q \), namely:

\[
p \Delta q = P \Delta Q + \Delta F - \frac{\partial F}{\partial t} \bigg|_{q,Q} \Delta t
\]

The Jacobian for the measure is unity, and the Hamiltonian conversion is equally trivial, since they are both local, and leads to:

\[
H = K + \frac{\partial F}{\partial t} \bigg|_{q,Q}
\]

Putting this all together leads to the sought after equality, namely:

\(^1\)It was the lack of a viscous term in our numerical experiment that lead to a \((\Delta t)^2\) error, as opposed to the more general \((\Delta t)^{3/2}\) error.
has a sensitivity to the order in which the path integral a well-defined object \cite{Daubechies and Klauder, 1985}. The phase space path integral also \cite{Chernoff, 1981; Kapoor, 1984; Dirac, 1925; 1958}. Such consiste ncy is part of the way to making the ical transformations. It permits a consistent (although not uniqu e) quantization of a classical system The utility of having a canonically invariant prescription for the path integral extends beyond just canon-

5 Corollaries

The utility of having a canonically invariant prescription for the path integral extends beyond just canonical transformations. It permits a consistent (although not unique) quantization of a classical system \cite{Chernoff, 1981; Kapoor, 1984; Dirac, 1925; 1958}. Such consistency is part of the way to making the path integral a well-defined object \cite{Daubechies and Klauder, 1985}. The phase space path integral also has a sensitivity to the order in which the \( p \) and \( q \) integrations are performed. This problem and its solution is discussed elsewhere \cite{Shiekh, 1990}.

It should be emphasised that the symmetric path integral is favoured (not compelled) over other prescriptions, in that it generates no anomalous additional terms during the canonical transformation. Note, however, that to get into and from this scheme, stochastic \((\hbar^2)\) terms appear. The virtue of no terms occurring during the transformation is that the Hamiltonian behaves well under the transformation, and is then (for example) trivialised by a Hamilton-Jacobi transformation.

6 Acknowledgments

I should like to thank ICTP for support during this work.

7 Appendix: Explicit Discretizations

The first three (Wick rotated) symmetric path integral discretizations with \( \hbar = 1 \) and end points held fixed (coherent state like path integral) are given by:

\[
\bar{I}_2 = \frac{1}{(4\pi)^2} \int_{-\infty}^{\infty} dq_1 dq_1 \int_{-\infty}^{\infty} dp_2 dp_2 \exp \left( \frac{i}{\hbar}(p_1 q_2 - q_0) - H(q_1, p_1, t_1) T/3 \right)
+ \frac{i}{2}(p_2(q_2 - q_1)) - H(q_2, p_2, t_2) T/3 \right) \tag{28}
\]

\[
\bar{I}_4 = \frac{1}{(4\pi)^4} \int_{-\infty}^{\infty} dq_1 dq_1 \int_{-\infty}^{\infty} dp_1 dp_4 \exp \left( \frac{i}{\hbar}(p_1(q_2 - q_0)) - H(q_1, p_1, t_1) T/5 \right)
+ \frac{i}{2}(p_2(q_2 - q_1)) - H(q_2, p_2, t_2) T/5 \right) \tag{29}
\]

\[
\bar{I}_6 = \frac{1}{(4\pi)^6} \int_{-\infty}^{\infty} dq_1 dq_0 \int_{-\infty}^{\infty} dp_1 .. dp_6 \exp \left( \frac{i}{\hbar}(p_1(q_2 - q_0)) - H(q_1, p_1, t_1) T/7 \right)
+ \frac{i}{2}(p_2(q_2 - q_1)) - H(q_2, p_2, t_2) T/7 \right) \tag{30}
\]

having restored the end integrals (at the cost of no error in the limit).

This completes the demonstration that the symmetric form canonically transforms cleanly.
These might be compared against the corresponding, more usual, discretizations given by:

\[ I_2 = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} dq_1 dq_1 \int_{-\infty}^{\infty} dp_2 dp_2 \exp \left( \begin{array}{l} ip_1(q_1 - q_a) - H(q_a, p_1)T/3 \\
+ip_2(q_2 - q_1) - H(q_1, p_2)T/3 \\
+ip_5(q_5 - q_2) - H(q_2, p_5)T/3 \end{array} \right) \]  

(31)

\[ I_4 = \frac{1}{(2\pi)^4} \int_{-\infty}^{\infty} dq_1 dq_4 \int_{-\infty}^{\infty} dp_1 dp_4 \exp \left( \begin{array}{l} ip_1(q_1 - q_a) - H(q_a, p_1)T/5 \\
+ip_2(q_2 - q_1) - H(q_1, p_2)T/5 \\
+ip_3(q_3 - q_2) - H(q_2, p_3)T/5 \\
+ip_5(q_5 - q_3) - H(q_3, p_5)T/5 \\
+ip_6(q_6 - q_5) - H(q_5, p_6)T/5 \end{array} \right) \]  

(32)

\[ I_6 = \frac{1}{(2\pi)^6} \int_{-\infty}^{\infty} dq_1 dq_6 \int_{-\infty}^{\infty} dp_1 dp_6 \exp \left( \begin{array}{l} ip_1(q_1 - q_a) - H(q_a, p_1)T/7 \\
+ip_2(q_2 - q_1) - H(q_1, p_2)T/7 \\
+ip_3(q_3 - q_2) - H(q_2, p_3)T/7 \\
+ip_4(q_4 - q_3) - H(q_3, p_4)T/7 \\
+ip_5(q_5 - q_4) - H(q_4, p_5)T/7 \\
+ip_6(q_6 - q_5) - H(q_5, p_6)T/7 \\
+ip_6(q_6 - q_5) - H(q_5, p_6)T/7 \end{array} \right) \]  

(33)

8 References

H. Goldstein, ‘Classical Mechanics’, (Addison-Wesley, Reading, MA, 2nd ed, (1980), 93-.

J. Gervais and A. Jevicki, “Point canonical transformations in the path integral”, Nucl. Phys. B 10, (1980), 93-.

J. Klauder, ‘Path Integrals’, Proceedings of the XIX. Internationale Universitätswochen für Kernphysik, Schladming, Austria, Acta Physica Austriaca, Suppl. XXII, (1980), 3-.

A. Anderson, ‘Quantum Canonical Transformations: Physical Equivalence of Quantum Theories’, Phys. Lett. B 305, (1993), 67-.

A. Anderson, ‘Quantum Canonical Transformations and Integrability: Beyond Unitarity Transformations’, Phys. Lett. B 319, (1993), 157-.

A. Anderson, ‘Canonical Transformations in Quantum Mechanics’, Ann. Phys. (NY) 232, (1994), 292-.

A. Anderson, ‘Special Functions from Canonical Transformations’, J. Math. Phys. 35, (1994), 6018-.

M. Swanson, ‘Canonical Transformations and Path Integral Measures’, to appear in Phy. Rev. A, (1994).

R. Feynman, ‘Space-Time Approach to Quantum Mechanics’, Rev. Mod. Phys. 20 (1948), 267-.

(reprinted in “Quantum Electrodynamics”, Ed. J.Schwinger, Dover, 1958.)

R. Feynman and A. Hibbs, “Quantum Mechanics and Path Integrals”, McGraw-Hill, (1965).

R. Fanelli, ‘Canonical Transformations and Phase Space Path Integrals’, J. Math. Phys., 17, (1976), 490-

L. Schulman, “Techniques and Applications of Path Integration”, Wiley, (1981).

I. Mayes and J. Dowker, ‘Canonical Functional Integrals in General Coordinates’, Proc. R. Soc. Lond., A.327, (1972), 131-.
I. Mayes and J. Dowker, ‘Hamiltonian Orderings and Functional Integrals’, J. Math. Phys., 14, (1973), 434-.

A. Shiekh, “Canonical transformations in quantum mechanics: A canonically invariant path integral”, J. Math. Phys., 29 (4), (1988), 913-.

I. Daubechies and J. Klauder, ‘True Measures for real time Path Integrals’, in “Path Integrals from meV to MeV”, Ed. M. Gutzwiller, A. Inomata, J. Klauder and L. Streit, World Scientific, (1985), 425-.

A. Shiekh, “The trivialization of constrains in quantum theory (working in a general gauge/parametrization)”, J. Math. Phys., 31 (1), (1990), 76-.

P. Chernoff, ‘Mathematical Obstructions to Quantization’, Had. J., 4, (1981), 879-.

A. Kapoor, ‘Quantization in Nonlinear Coordinates via Hamiltonian Path Integrals’, Phys.Rev., D 29, (1984), 2339-.

P. Dirac, ‘The Fundamental Equations of Quantum Mechanics’, Proc. Roy. Soc. A 109, (1925), 642-.

P. Dirac, “The Principles of Quantum Mechanics”, 4th Ed., Oxford, (1958).