Canonical transformations and path-integral measures

Mark S. Swanson
Department of Physics, University of Connecticut, Stamford, Connecticut 06903
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This paper is a generalization of previous work on the use of classical canonical transformations to evaluate Hamiltonian path integrals for quantum-mechanical systems. Relevant aspects of the Hamiltonian path integral and its measure are discussed, and used to show that the quantum-mechanical version of the classical transformation does not leave the measure of the path-integral invariant, instead inducing an anomaly. The relation to operator techniques and ordering problems is discussed, and special attention is paid to incorporation of the initial and final states of the transition element into the boundary conditions of the problem. Classical canonical transformations are developed to render an arbitrary power potential cyclic. The resulting Hamiltonian is analyzed as a quantum system to show its relation to known quantum-mechanical results. A perturbative argument is used to suppress ordering-related terms in the transformed Hamiltonian in the event that the classical canonical transformation leads to a nonquadratic cyclic Hamiltonian. The associated anomalies are analyzed to yield general methods to evaluate the path integral's prefactor for such systems. The methods are applied to several systems, including linear and quadratic potentials, the velocity-dependent potential, and the time-dependent harmonic oscillator.

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I. INTRODUCTION

The relationship between classical mechanics and its quantum counterpart is nowhere more evident than in the path-integral formulation of transition amplitudes [1–3], where the classical action evaluated along a possible trajectory appears as a weighting phase factor for the trajectory. In the Hamiltonian form for the path integral the classical action appears, at least formally, written in terms of the canonically conjugate variables q and p. In classical mechanics it is precisely this form of the action that is used to define canonical transformations [4] to new canonical variables, i.e., those that preserve the Poisson bracket structure. With an appropriate choice of canonical transformation the classical action can be transformed to cyclic coordinates or, in the case of the Hamilton-Jacobi equation, the Hamiltonian can be transformed identically to zero. At the classical level the solution of Hamilton's equations becomes trivial for such a Hamiltonian.

For certain transition elements the measure of the corresponding Hamiltonian path-integral is symmetric in its integrations over intermediate p and q values and is therefore invariant under a transformation that has a Jacobian of unity. Since the Poisson bracket of a canonical transformation is identical to the inverse Jacobian of the transformation, a canonical transformation apparently introduces no factors into the measure. At first glance it would then seem that the classical canonical transformation to cyclic variables could be applied to the Hamiltonian path integral to render it exactly integrable, thus providing a method for nonperturbative analysis of transition elements. Further analysis reveals that the transformed path integral yields results differing from those of the original untransformed path integral, and indeed those of other methods such as wave mechanics. In particular, the time-dependent prefactor or, loosely speaking, the van Vleck determinant [5] is incorrectly calculated using this method. The loss of such information is catastrophic to understanding the thermal behavior, the stability, and tunneling rates of the system. Perhaps more disturbing, the invariance of the Hamiltonian path-integral measure under canonical transformations is a central assumption in the path-integral method for implementing first and second class constraints [6,7], a method whose generalization to gauge theories was seminal to their quantization. Recently developed equivariant localization techniques [8] also rely on the ability to transform the Hamiltonian path integral to new coordinates while introducing no unexpected terms in the measure.

The problem, as discussed by numerous authors [9–14], lies in the action appearing in the path integral. The time derivatives appearing in the path-integral action are *formal* identifications only, behaving like the derivative familiar from calculus only for certain systems. As a result, the classical canonical transformation does not have the same result when it is applied to the path-integral action, and in fact it induces additional terms into the action. An alternative approach to canonical transformations for the path integral is to define a quantum-mechanical version of the canonical transformation that is consistent with the formal time derivatives of the path integral [15,16]. Such an approach will be followed in this paper. However, this quantum canonical transformation neither leaves the measure invariant, instead inducing nontrivial Jacobians, nor necessarily reproduces the classical result for the transformed Hamiltonian. In a previous paper that concentrated on the measure [16] it was shown that the induced Jacobians could be absorbed into the action of the path integral where they appear as $O(\hbar)$ terms. Alternatively, the Jacobian was shown to be equivalent to a time-dependent prefactor that reproduced the van Vleck determinant of the original path integral, at least for the case of the simple harmonic oscillator. This paper will consider both aspects of quantum canonical transformations and generalize the previous results, fleshing out derivations along the way. In addition, results regarding the application of canonical transformations to the path integral as well as relevant properties of the path integral will be presented and demonstrated for various systems.

The outline of this paper is as follows. In Sec. II the quantum-mechanical transition element to be analyzed will be expressed as a Hamiltonian path integral. Certain properties of expectation values necessary to the remainder of the paper will be derived from this path integral for general cases of the Hamiltonian. The relation of the initial and final states to the boundary values of Hamilton's equations is discussed, since this will be of importance to the quantum canonical transformation. It is shown that there exist classically suppressed potentials, i.e., ones that would not contribute to the classical variation of the action, that contribute $O(\hbar)$ terms to the quantum-mechanical action. Poisson resummation techniques are applied to path integrals with periodic boundary conditions, such as the square well system, to transform the measure to continuous variables. The relation of continuum techniques to the boundary conditions is discussed for the Hamiltonian path integral. In Sec. III the classical canonical transformation will be reviewed with special attention to the relation of the surface or end point terms generated by the canonical transformation to the boundary conditions of the transition element. The operator ordering ambiguities associated with the quantum-mechanical version of these transformations are briefly discussed and the specific problem of Cartesian versus polar coordinates is used to demonstrate them. A classical canonical transformation to cyclic coordinates is derived for the case of an arbitrary power potential. The resulting classical Hamiltonian is analyzed as a quantum-mechanical problem, thereby ignoring the ordering ambiguities present in the transformation. The results are shown to correspond to the correct energy spectrum for the cases that the parent Hamiltonian constituted a solvable problem. Section IV begins by examining the ramifications for the path integral of assuming the existence of new canonically conjugate variables. A consistency condition for this change of variables is derived from the demand for a unit projection operator. The quantum canonical transformation is introduced in terms of a generating function and the forms of the new variables are derived. The consistency condition is found to be related to the problem of initial and final conditions for the new variables, and some of the limitations of the quantum canonical transformation are revealed. From the form of the new variables the explicit form for the Jacobian or anomaly of the transformation is calculated, and its incorporation into the action of the path integral is shown. For a general form of the generating function the anomaly itself is shown to be a surface term, contributing to the overall prefactor or van Vleck determinant. The form of the transformed Hamiltonian is discussed, and a perturbative proof of the suppression of ordering terms for a cyclic Hamiltonian is given. In Sec. V various systems, some known exactly by other methods, are evaluated. These include the velocity-dependent transformation of the free particle, the linear potential, the transition from Cartesian to polar coordinates, and the harmonic oscillator. Finally, the results are extended to give an approximate solution to the important case of the time-dependent harmonic oscillator.

II. THE HAMILTONIAN PATH INTEGRAL

In this section several aspects of Hamiltonian path integrals that are relevant to developments later in this paper will be discussed. While these aspects may appear at first blush to be unrelated, they will be important later in this paper to understanding the consequences of canonically transforming the variables of integration in the path integral.

A. Defining the Path Integral

The transition element to be analyzed in the remainder of this paper is given in its one-dimensional form by

$$W_{fi} = \langle p_f \,|\exp(-i\hat{H}T/\hbar)|\, q_i \rangle \,. \tag{1}$$

The final state $|\, p_f \rangle$ is assumed to be an eigenstate of the momentum $\hat{p}$, while the initial state $|\, q_i \rangle$ is an eigenstate of the position $\hat{q}$. The two operators satisfy the usual algebra $[\hat{q},\hat{p}] = i\hbar$. The Hamiltonian $\hat{H}$ is assumed to be a function of some ordering of $\hat{q}$ and $\hat{p}$, and its eigenstates, as well as those of $\hat{q}$ and $\hat{p}$, are determined consistent with any boundary conditions, such as periodicity in q.

W_{fi} is trivial to evaluate if $\hat{H}$ is cyclic, i.e., a function solely of $\hat{p}$. For such a case it reduces to

$$W_{fi} = \langle p_f \,|\, q_i \rangle \, \exp\left[-iH(p_f)T/\hbar\right] . \tag{2}$$

The allowed values of the variables p_f and q_i appearing in the inner product in (2) are determined by the boundary conditions of the original problem, although in one dimension the inner product for continuous systems takes the general form

$$\langle p_f \,|\, q_i \rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left(-ip_f q_i/\hbar\right) . \tag{3}$$

The propagator of the quantum-mechanical problem can be derived from result (1). Assuming that the momentum state spectrum is continuous, the propagator is obtained by a Fourier transform,

$$\langle q_f \,|\exp(-i\hat{H}T/\hbar)|\, q_i \rangle = \int \frac{dp_f}{\sqrt{2\pi\hbar}}\, e^{ip_f q_f/\hbar} \langle p_f \,|\exp(-i\hat{H}T/\hbar)|\, q_i \rangle \,. \tag{4}$$

Obviously, a discrete spectrum of momentum eigenstates leads to a Fourier series. Once the propagator (4) is known, results such as the ground state energy can be derived.

The Hamiltonian path-integral representation of (1) may be derived by using the completeness of the position and momentum eigenstates to perform a time-slicing argument. This technique is well documented [3], and its application here is accomplished by using the unit projection operator given by

$$\hat{1} = \int \frac{dp_j}{\sqrt{2\pi\hbar}}\, dq_{j+1}\,|\,q_{j+1}\,\rangle e^{iq_{j+1}p_j/\hbar}\langle\, p_j\,|\,. \qquad (5)$$

There is an important subtlety in (5). As it is written it assumes that the spectra of the states are continuous; however, this will not be the case in the event that the configuration space of the system is compact or periodic. Putting aside such a possibility for the moment, the result of time slicing T into N intervals of duration ϵ, where $\epsilon = T/N$, gives

$$\langle\, p_j\,|\exp(-i\epsilon\hat{H}/\hbar)|\,q_j\,\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp\left\{-\frac{i}{\hbar}\left[q_jp_j + \epsilon H(p_j,q_j) + O(\epsilon^2)\right]\right\}, \qquad (6)$$

where the $O(\epsilon^2)$ terms arise from commutators occurring in the ordering of the Hamiltonian power series. This immediately yields the Hamiltonian path-integral recipe for calculating the transition amplitude:

$$W_{fi} = \langle\, p_f\,|e^{-iHT/\hbar}|\,q_i\,\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int\prod_{j=1}^{N}\frac{dp_j}{2\pi\hbar}\,dq_j\,\exp\left\{\frac{i}{\hbar}\sum_{j=1}^{N}[-q_j(p_{j+1}-p_j) -\epsilon H(p_j,q_j)] - \frac{i}{\hbar}q_ip_1\right\}, \qquad (7)$$

where $p_{N+1} = p_f$ and the limits $N \to \infty$ and $\epsilon \to 0$ are understood.

B. The leading behavior of Δq

It is standard practice to assume a continuous form for the path integral by identifying $\epsilon \to dt$ and $q_j(p_{j+1} - p_j) = dt\, q_j\, \dot{p}_j$. The latter identification is *purely formal*, since p_{j+1} and p_j are independent variables of integration unrelated by any time evolution. Even with this formal identification the action density in the path integral (7) can take the (semi)standard form, $-q\dot{p}-H$, only if $p_i = 0$ or $q_i = 0$. For these cases the final term can be written $-iq_i(p_1 - p_i)$. This will be discussed in greater detail in Sec. IV. Another technicality arises since the argument of the path integral does not satisfy the criteria of a probability measure unless the time is continued to imaginary values, the so-called Wick rotation. Otherwise the oscillatory integrands result in distributions rather than functions. The Wick rotation will be used and assumed to yield a sensible measure for all path integrals considered in the remainder of this paper.

To demonstrate the formal nature of the identification $q_j(p_{j+1} - p_j) = dt\, q_j\, \dot{p}_j$ as well as derive results that will be important later in this paper, it will be of use to discuss the leading behavior in ϵ of the expectation value of the element $\Delta q_j = q_{j+1} - q_j$. For it to be possible to treat Δq_j as $\dot{q}\, dt$ its expectation value $\langle\Delta q_j\rangle_{fi}$ must be shown to be $O(\epsilon)$. The behavior of $\langle\Delta q_j\rangle$ is of course a function of the specific form of the Hamiltonian. However, if the Hamiltonian is cyclic, then it is always true that $\langle\Delta q_j\rangle_{fi}$ is $O(\epsilon)$. This is easy to demonstrate within the operator context, where the operator form for Hamilton's equation gives

$$\Delta\hat{q}(t) = \hat{q}(t+\epsilon) - \hat{q}(t) = \epsilon\,\frac{i}{\hbar}[\hat{H}(\hat{p}),\hat{q}(t)] = \epsilon\,\frac{\partial\hat{H}(\hat{p})}{\partial\hat{p}}\,. \qquad (8)$$

Inserting (8) into (1) and using (2) immediately yields

$$\langle\Delta\hat{q}(t)\rangle_{fi} = \epsilon\,\langle\, p_f\,|\,q_i\,\rangle\,\frac{\partial H(p_f)}{\partial p_f}\exp[-iH(p_f)\,T/\hbar]\,. \qquad (9)$$

Demonstrating the path-integral equivalent of result (9) requires adding a source term $K_j\Delta q_j$ to the action. In order to avoid difficulties with the boundary conditions on q_j, the boundary conditions $K_N = K_0 = 0$ are imposed on the source function. The expectation value is then given by

$$\langle\Delta q_j\rangle_{fi} = -\left.\frac{i}{\hbar}\frac{\partial W_{fi}[K]}{\partial K_j}\right|_{K=0}\,. \qquad (10)$$

The next step is to perform the path-integral version of integrating by parts by using the boundary condition on K to rearrange the sum over j:

$$\sum_{j=1}^{N}K_j\Delta q_j = \sum_{j=1}^{N}K_j(q_{j+1}-q_j) = -\sum_{j=1}^{N}q_j(K_j - K_{j-1}) \equiv -\sum_{j=1}^{N}q_j\Delta K_j\,. \qquad (11)$$

Since H depends only on p all q integrations can now be performed. Assuming that the range of the q integrals is $\pm\infty$, each of the N integrations over q yields a Dirac delta,

$$\int dq_j\,\exp\left\{-\frac{i}{\hbar}q_j(p_{j+1}-p_j+\Delta K_j)\right\} = 2\pi\hbar\,\delta(p_{j+1}-p_j+\Delta K_j)\,. \qquad (12)$$

The p variables are now trivial to integrate, giving the result for the transition element

$$W_{fi}[K] = \frac{1}{\sqrt{2\pi\hbar}} \exp\left\{ -\frac{i}{\hbar} \left(p_f q_i + \sum_{j=1}^{N} \epsilon H(p_f - K_{j-1}) \right) \right\} . \quad (13)$$

Using (13) in (10), along with the result that

$$\lim_{N\to\infty} \sum_{j=1}^{N} \epsilon = T , \quad (14)$$

reproduces the operator result (9):

$$\lim_{N\to\infty} \langle \Delta q_j \rangle_{fi} = \frac{\epsilon}{\sqrt{2\pi\hbar}} \frac{\partial H(p_f)}{\partial p_f} \times \exp\left\{ -\frac{i}{\hbar} [p_f q_i + H(p_f)T] \right\} . \quad (15)$$

Result (15) does not necessarily follow for noncyclic Hamiltonians. The argument used to derive (15) can be applied to the harmonic oscillator action to show that $\langle (\Delta q_j)^2 \rangle_{fi}$ is $O(\epsilon)$. This is easily seen from the Gaussian nature of the Wick-rotated integrations. The q integration results in

$$\int dq_j \exp\left[-\epsilon \frac{1}{2} q_j^2 + q_j(\Delta K_j + \Delta p_j) \right] = \sqrt{\frac{2\pi}{\epsilon}} \exp\left[-\frac{(\Delta p_j + \Delta K_j)^2}{\epsilon} \right] . \quad (16)$$

The ΔK_j dependence may be removed from this term by translating the p_j variables according to $p_j \to p_j + K_j$. Doing so changes the p_j^2 term in the exponential of the path integral according to

$$-\epsilon \frac{1}{2} p_j^2 \to -\epsilon \frac{1}{2} p_j^2 - \epsilon p_j K_j - \epsilon \frac{1}{2} K_j^2 . \quad (17)$$

It is then clear that the second derivative of the resulting function with respect to K_j will result in a term $O(\epsilon)$. In an identical manner it is possible to show that the expectation value of $\Delta p_j = p_{j+1} - p_j$ vanishes if the Hamiltonian is cyclic. This is the quantum-mechanical equivalent of the classical Hamilton equation

$$\dot{p} = -\frac{\partial H}{\partial q} . \quad (18)$$

As a result of (15) it is possible to use a perturbative argument to show that certain types of terms in the Hamiltonian of the path integral are suppressed in the limit $N \to \infty$. The Hamiltonian under consideration has the form

$$H = H_{\rm cl}(p,q) + H_\Delta(\Delta q, q) , \quad (19)$$

where all terms in H_Δ have at least one positive power of Δq and $H_{\rm cl}$ is the Hamiltonian inherited from the classical system. Such a Hamiltonian has no classical counterpart, since terms of the form H_Δ would be suppressed [13]. If $H_{\rm cl}$ is cyclic it can be shown that the terms H_Δ do not contribute to the path integral in the limit $N \to \infty$. The argument is similar to the one used to demonstrate (15). The contribution of the terms H_Δ is written as a perturbation series using $H_{\rm cl}$ as the basis Hamiltonian. This is accomplished by adding the source terms $\epsilon K_j \Delta q_j$ and $\epsilon J_j q_j$ to the action without H_Δ to give the function $W_{fi}[K, J]$. The perturbation series representation of the original transition element is then defined as

$$\exp\left\{ -\frac{i}{\hbar} \sum_{j=1}^{N} \epsilon H_\Delta \left(\frac{\hbar}{i\epsilon} \frac{\partial}{\partial K_j}, \frac{\hbar}{i\epsilon} \frac{\partial}{\partial J_j} \right) \right\} W_{fi}[K, J] \Bigg|_{K,J=0} . \quad (20)$$

The function $W_{fi}[K, J]$ is readily evaluated to give

$$W_{fi}[K] = \frac{1}{\sqrt{2\pi\hbar}} \exp\left\{ -\frac{i}{\hbar} \left[p_f q_i + \sum_{j=1}^{N} \epsilon H\left(p_f - \epsilon K_{j-1} - \sum_{l=1}^{j} \epsilon J_l \right) \right] \right\} . \quad (21)$$

While the $\sum \epsilon J$ term results in an integral in the limit $\epsilon \to 0$, it is clear that the term ϵK is suppressed relative to the other terms by a factor of T/N. The derivatives with respect to K are suppressed by this factor as well, showing that terms of the form H_Δ do not contribute to the perturbation series. For the case that the basis Hamiltonian is cyclic such terms can therefore be discarded. In effect, this perturbative argument substantiates the general intuition that, for a cyclic Hamiltonian, Δq can be replaced by $\epsilon \dot{q}$, where $\dot{q}$ is finite. Any resulting terms with factors of $O(\epsilon^2)$ or greater can then be suppressed.

Since perturbative arguments are fraught with pitfalls and loopholes, it is worth checking this result for exactly integrable cases. For example, the path integral whose Hamiltonian is given by

$$H = \frac{1}{2} p^2 + \lambda q \Delta q \quad (22)$$

can be shown to reduce to the standard cyclic result (2) with all terms proportional to λ suppressed by an additional factor of ϵ^2. Terms of the form $q\Delta p$ or $p\Delta p$ can be integrated exactly to find the standard cyclic result in the limit $\epsilon \to 0$. However, there is at least one important set of cases not covered by this perturbative argument involving terms with quadratic powers of p. For example, if the term $f(q)\Delta q p^2$ occurs in the Hamiltonian, its contribution cannot be discarded. It is not difficult to see the mechanism for this by examining the Hamiltonian

$$H = \frac{1}{2} p^2 + \frac{1}{2} \Delta q f(q) p^2 = \frac{1}{2} [1 + f(q)\Delta q] p^2 . \quad (23)$$

The p integrations in the Wick-rotated path integral are

Gaussian, and take the general form

$$\int \frac{dp_j}{2\pi\hbar} \exp\left\{-\frac{\epsilon}{\hbar}\left[\frac{1}{2}[1+f(q_j)\Delta q_j]p_j^2 - p_j\frac{\Delta q_j}{\epsilon}\right]\right\}$$

$$= \sqrt{\frac{1}{2\pi\hbar\epsilon[1+f(q_j)\Delta q_j]}} \exp\left[\frac{(\Delta q_j)^2}{2\hbar\epsilon[1+f(q_j)\Delta q_j]}\right] . \tag{24}$$

If Δq remains proportional to some positive power or root of ϵ, then the Δq term in the denominator of the exponential can be discarded due to the factor of ϵ present in the denominator. However, the terms in the prefactor may contribute to the path integral. This follows from the fact that the prefactor terms can be written

$$\frac{1}{\sqrt{1+f(q_j)\Delta q_j}} = \exp\left[-\frac{1}{2}\ln[1+f(q_j)\Delta q_j]\right]$$

$$\approx \exp\left[-\frac{1}{2}f(q_j)\Delta q_j\right] . \tag{25}$$

Even if $\Delta q_j \approx \epsilon$, the infinite sum in which (25) becomes embedded can result in a nontrivial contribution since $N\epsilon \to T$. The upshot of result (25) is to transmute the original interaction term $f(q)\Delta q\, p^2$ into an effective velocity-dependent potential in the path integral when all momenta have been integrated. This velocity-dependent potential appears proportional to $\hbar$, since (24) can be written

$$\sqrt{\frac{1}{2\pi\hbar\epsilon[1+f(q_j)\Delta q_j]}} \exp\left[\frac{(\Delta q_j)^2}{2\hbar\epsilon[1+f(q_j)\Delta q_j]}\right]$$

$$\approx \sqrt{\frac{1}{2\pi\hbar\epsilon}} \exp\left\{\frac{\epsilon}{\hbar}\left[\frac{1}{2}\dot{q}^2 + \frac{1}{2}\hbar f(q)\dot{q}\right]\right\} , \tag{26}$$

where the standard path-integral notation $\Delta q = \epsilon\dot{q}$ has been used. Result (26) is consistent with the idea that the classical Hamiltonian (23) would receive no contribution from such a potential. If it is to give a nontrivial contribution to the quantum-mechanical theory, it must be equivalent to a term in the action of $O(\hbar)$ or higher. Clearly, similar results can be obtained for other Gaussian-like terms for specific choices of the cyclic Hamiltonian. A discussion of possible terms that may contribute is given by Prokhorov [13].

It is worth noting for later reference that, if the Hamiltonian is cyclic, the path integral (7) can be evaluated exactly by translating the variables of integration by the classical solutions to Hamilton's equations consistent with the boundary conditions $q(t=0) = q_i$ and $p(t=T) = p_f$, given by

$$p_c(t) = p_f\ , \quad q_c(t) = q_i + \frac{\partial H(p_f)}{\partial p_f}t\ . \tag{27}$$

This is possible because the difference between adjacent time slices *does* reduce to the derivative for a classical function, i.e., $q_c(t_{j+1}) = q_c(t_j+\epsilon) \to q_c(t_j) + \epsilon\dot{q}_c(t_j)$. Performing an integration by parts similar to (11) reduces the translated path integral (7) to

$$\frac{1}{\sqrt{2\pi\hbar}} \exp\left\{-\frac{i}{\hbar}[p_f q_i + H(p_f)T]\right\} \int \prod_{j=1}^{N} \frac{dp_j}{2\pi\hbar}\, dq_j \exp\left\{\frac{i}{\hbar}\sum_{j=1}^{N}\left[-q_j(p_{j+1}-p_j) - \epsilon\frac{1}{2}p_j^2\frac{\partial^2 H(p_c(t_j))}{\partial p_c(t_j)^2} - \cdots\right]\right\} , \tag{28}$$

where the ellipsis refers to higher-order terms present in the expansion of $H(p_c(t_j)+p_j)$ around p_j and, because of the translation of variables, $p_{N+1} = 0$. It is precisely the latter result that reduces the translated path integral appearing in (28) to unity when all integrations are performed, a fact that is apparent when result (12) is examined for the case $K = 0$. Therefore the only surviving factor in (28) is the exponential of the classical action evaluated along the classical trajectory (27).

C. Discrete spectrum path integrals

Another relevant point regards the case where the allowed values of the momentum or energy constitute a denumerably infinite set rather than a continuous variable. Such a result is common in quantum-mechanical systems, occurring in bound state spectra and in systems where the configuration space is compact or periodic boundary conditions are enforced. In wave mechanics the discrete spectrum can arise from demanding either that the bound state wave function is normalizable or that the wave function or its derivative vanishes on some boundaries. It is natural to expect that the measure of the path integral for such a system would differ from its "free" counterpart (7). However, it is often the case that the path-integral representation of the transition amplitude (1) for such a system is identical to the continuous result (7). This outcome is well known within the context of specific systems [17]. Since this aspect of path integrals is relevant to canonical transformations, the general derivation of the range of integrations will be sketched for the specific case of a *free* particle constrained to be in a one-dimensional infinite square well.

The position eigenstates range from $-a$ to a, while the momentum eigenstates $|n\rangle$ are discrete and indexed by an integer n. Unit projection operators are given by

$$\hat{1} = \int_{-a}^{a} dq\,|q\rangle\langle q|\ , \quad \hat{1} = \sum_{n=-\infty}^{\infty} |n\rangle\langle n|\ , \tag{29}$$

while the inner product is given by

$$\langle q \mid n \rangle = \frac{1}{\sqrt{2a}} \exp\left(\frac{i\pi n q}{a}\right) . \tag{30}$$

Of course, the physical energy eigenstates are linear combinations of $| n \rangle$ and $| -n \rangle$ consistent with the boundary conditions. The time-slicing argument that was used to construct (7) can be revisited using (29) and (30) to obtain

$$\begin{aligned} W_{fi} &= \langle n_f | e^{-i\hat{H}T/\hbar} | q_i \rangle \\ &= (2a)^{-(N+1)/2} \sum_{n_1,\ldots,n_N} \int_{-a}^{a} dq_1 \cdots dq_N \exp\left\{ -\frac{i}{\hbar} \sum_{j=1}^{N} \left[\frac{n_j \pi \hbar}{a}(q_j - q_{j-1}) - \epsilon H(n_j) \right] - \frac{i n_f \pi q_N}{a} \right\} , \end{aligned} \tag{31}$$

where $q_0 = q_i$.

Result (31) can be rewritten using the Poisson resummation technique, which begins by using the identity

$$\sum_{n=-\infty}^{\infty} f(n) = \sum_{k=-\infty}^{\infty} \int_{-\infty}^{\infty} dn\, f(n)\, e^{i2\pi kn} . \tag{32}$$

Using (32) and making the obvious definition $p_j = n_j \pi \hbar / a$ allows (31) to be written as

$$W_{fi} = \frac{1}{\sqrt{2a}} \int_{-\infty}^{\infty} \frac{dp_1}{2\pi\hbar} \cdots \frac{dp_N}{2\pi\hbar} \int_{-a}^{a} dq_1 \cdots dq_N \sum_{k_1,\ldots,k_N} \exp\left\{ -\frac{i}{\hbar} \sum_{j=1}^{N} [p_j(q_j + 2ak_j - q_{j-1}) - \epsilon H(p_j)] - \frac{i}{\hbar} p_f q_N \right\} . \tag{33}$$

Because the Hamiltonian is independent of q and the sums over the k_j are infinite, the sums may be absorbed by extending the range of the q_j integrations. However, this is contingent on the fact that

$$\exp\left\{ -\frac{i}{\hbar} p_f (q_N + k_N 2a) \right\} = \exp\left\{ -\frac{i}{\hbar} p_f q_N \right\} , \tag{34}$$

which holds as long as $p_f = n_f \pi \hbar / a$ and n_f is an integer. Because the wave-mechanical solution to the problem was used to derive the path-integral form, it is clear that condition (34) holds. The final form of the path integral is given by

$$\begin{aligned} W_{fi} = \frac{1}{\sqrt{2a}} \int_{-\infty}^{\infty} \frac{dp_1}{2\pi\hbar} \cdots \frac{dp_N}{2\pi\hbar} dq_1 \cdots dq_N \\ \times \exp\left\{ -\frac{i}{\hbar} \sum_{j=1}^{N} [q_j(p_{j+1} - p_j) - \epsilon H(p_j)] \right. \\ \left. - \frac{i}{\hbar} p_1 q_i \right\} , \end{aligned} \tag{35}$$

where the limits on the q_j integrations are now $\pm\infty$. Apart from the overall factor of $(2a)^{-1/2}$, result (35), with its ambiguous symbol $p_{N+1} = p_f$, is formally identical in its measure and action to the free case (7). In that sense information about the system has been lost in the transition from (31) to (35) since the form (35) does not specify a discrete spectrum for p_f. *A priori* knowledge of the momentum spectrum is required in order that the discrete form of the Fourier transform, rather than the continuous form, is employed to obtain the propagator (4).

D. Fourier methods for evaluating path integrals

A final aspect of importance regarding the Hamiltonian path integral is the method that does allow the action in the path integral to be manipulated as if the formal time derivative was a true derivative. The q_j and p_j variables are first translated by a classical solution to Hamilton's equations of motion consistent with the boundary conditions. This means using classical solutions for both p and q that satisfy the conditions

$$p_c(t = T) = p_f , \quad q_c(t = 0) = q_i . \tag{36}$$

Because there is no initial condition for p or final condition for q in the original form of the transition element, the translated p and q variables do not necessarily vanish at *both* $t = 0$ and $t = T$. Consistent with these boundary conditions, the $2N$ fluctuation variables q_j and p_j are written as Fourier expansions in terms of $2N$ new variables q_n and p_n,

$$q_j = \sum_{n=0}^{N-1} q_n \sin\left(\frac{(2n+1)\pi t_j}{2T}\right) , \tag{37}$$

$$p_j = \sum_{n=0}^{N-1} p_n \left(\frac{(2n+1)\pi}{2T}\right) \cos\left(\frac{(2n+1)\pi t_j}{2T}\right) . \tag{38}$$

The expansions of (37) satisfy the proper translated quantum boundary conditions $p(t = T) = 0$ and $q(t = 0) = 0$, but are arbitrary at the remaining end points in order to accommodate the quantum nature of the coordinates. This is an outgrowth of the uncertainty principle for canonical variables, since the uncertainty principle forces q_f to be undefined if p_f is exactly known, with a similar relation between q_i and p_i. However, the formal derivatives in the path integral now become true derivatives, since to $O(\epsilon)$

$$q_{j+1} - q_j \to \epsilon \sum_{n=1}^{N} q_n \frac{(2n+1)\pi}{2T} \cos\left(\frac{(2n+1)\pi t_j}{2T}\right) . \quad (39)$$

The measure is rewritten in terms of integrations over the coefficients of the Fourier expansions. This change of variables is accompanied by a Jacobian that is nontrivial, but one that can be inferred by forcing the new path integral to yield the same results as the configuration space measure version discussed in the preceding part of this section. In addition to the usual Wick rotation $T \to -iT$, the Hamiltonian path integral also requires $p_n \to -ip_n$. The case of an arbitrary cyclic Hamiltonian is particularly easy since the integrations over the q_n variables yield a factor of the form

$$\left(\frac{8T}{\pi^2}\right)^N \prod_{n=0}^{N-1} (2n+1)^{-2} \delta(p_n) , \quad (40)$$

from which the Jacobian is inferred to be

$$J = \left(\frac{\pi^2}{8T}\right)^N [(2N-1)!!]^2 . \quad (41)$$

The validity of this procedure can be tested on the harmonic oscillator transition element. There the classical solutions consistent with the boundary conditions are

$$q_c(t) = A\sin(\omega t + \delta) , \quad p_c(t) = m\omega A\cos(\omega t + \delta) , \quad (42)$$

where

$$A = q_i \csc\delta , \quad \cot\delta = \frac{p_f \sec(\omega T)}{m\omega q_i} - \tan(\omega T) . \quad (43)$$

Using (42) and (43) in the harmonic oscillator action yields the result

$$\int_0^T dt\, \mathcal{L} = q_i p_f \sec(\omega T) - \frac{1}{2} m\omega q_i^2 \tan(\omega T) - \frac{1}{2}\frac{p_f^2}{m\omega} \tan(\omega T) . \quad (44)$$

The remaining translated action reduces to Gaussians in both p_n and q_n. Performing the integrations, combining the result with the Jacobian (41), and undoing the Wick rotation yields the prefactor

$$\lim_{N\to\infty} \prod_{n=0}^{N-1} \left(1 - \frac{4\omega^2 T^2}{(2n+1)^2}\right)^{-\frac{1}{2}} = \frac{1}{\sqrt{\cos\omega T}} . \quad (45)$$

Combining results (44) and (45) yields the correct form for the transition element (1) for the harmonic oscillator. In Sec. IV the ramifications of the quantum nature of the coordinate fluctuations for the boundary conditions of the canonically transformed coordinates will be discussed, and the results of this subsection will be used to define restrictions on the validity of the canonically transformed path integral.

III. CANONICAL TRANSFORMATIONS

A classical canonical transformation is one from the coordinates (q,p) to a new set of coordinates (Q,P) such that the Poisson bracket structure, or equivalently the volume of phase space, is preserved. For convenience and consistency only canonical transformations of the third kind [4] will be considered in the remainder of this paper, and these are defined by a choice for the generating function of the general form $F(p,Q,t)$. At the classical level the new variables are determined by solving the system of equations given by

$$q = -\frac{\partial F(p,Q,t)}{\partial p} , \quad P = -\frac{\partial F(p,Q,t)}{\partial Q} . \quad (46)$$

It is important to remember that Q and p are treated as independent in the definitions of the new coordinates given by (46). However, the proof that the Poisson bracket structure is preserved depends on the identities obtained by differentiating (46) and using the fact that $Q = Q(q,p)$. For example, it follows that

$$1 = \frac{\partial q}{\partial q} = -\frac{\partial^2 F(p,Q,t)}{\partial Q\, \partial p} \frac{\partial Q(q,p,t)}{\partial q} . \quad (47)$$

It is assumed that the equations of (46) are well defined and can be solved to yield $Q(q,p,t)$ and $P(q,p,t)$, or inverted to obtain $q(Q,P,t)$ and $p(Q,P,t)$. The action is transformed according to

$$\begin{aligned} &\int_0^T dt\, [-q\dot{p} - H(p,q)] \\ &= \int_0^T dt \left[P\dot{Q} - \tilde{H}(P,Q) + \frac{dF}{dt}\right] \\ &= F(p_f,Q_f,t_f) - F(p_i,Q_i,t_i) + \int_0^T dt\, [P\dot{Q} - \tilde{H}(P,Q)] , \end{aligned} \quad (48)$$

where

$$\tilde{H}(P,Q) = H(p(Q,P,t), q(Q,P,t)) + \frac{\partial F(p(P,Q),Q,t)}{\partial t} . \quad (49)$$

At the classical level there is no difficulty in obtaining initial and final values for both variables q and p since it is assumed that Hamilton's equations can be solved to obtain classical solutions consistent with any possible pair of boundary conditions over the arbitrary time interval T. The two unspecified end point values of the variables are simply those given by the classical solutions at the respective end point times. However, if canonical transformations are to be employed in a path-integral setting in a manner similar to the classical result, it is necessary to deal with the quantum-mechanical version of this problem, and there is no *a priori* reason to expect that the classical definition is consistent with the quantum-mechanical transition amplitude (1). This will be discussed in detail in Sec. IV.

It is apparent at the classical level that the values of the generating function evaluated at the end points, i.e., the surface terms, correspond to a piece of the minimized original classical action not determined by the minimized transformed action. This is demonstrated by examining the well-known canonical transformation to cyclic coordinates for the harmonic oscillator. Using the generating function

$$F(p,Q) = -\frac{p^2}{2m\omega}\tan Q \tag{50}$$

gives

$$Q = \arctan\frac{m\omega q}{p}\,, \quad \omega P = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2\,, \tag{51}$$

so that the transformed Hamiltonian is $\tilde{H} = \omega P$. It follows that the transformed action vanishes when evaluated along the classical trajectory $Q_c = \omega t + Q_i$ and $P_c = P_f = P_i$. Therefore the value of the original action along the classical trajectories q_c and p_c is contained entirely in the end point contributions of the generating function. An explicit calculation using the classical solutions (42) in (50) with $Q_i = \delta$ and $Q_f = \omega T + \delta$ verifies that the generating function end point values reproduce result (44). Because the value of the action along the classical trajectory is the phase of the quantum transition amplitude (1) in the WKB approximation, the value of knowing the form of the generating function for a canonical transformation to cyclic coordinates becomes apparent. Such a classical generating function already gives considerable information regarding the quantum transition amplitude.

However, it is important to note that the choice of ω appearing in the transformed Hamiltonian $\tilde{H}$ is arbitrary. Using the generating function

$$F(p,Q) = -\frac{p^2}{2m\omega}\tan\left(\frac{\omega}{\omega'}Q\right) \tag{52}$$

transforms the Hamiltonian to $\omega' P$. While the solution for Q becomes $Q = \omega' t + Q_i$, this has no effect on the solution for the original variable q because of the offsetting factors in the generating function. This is merely a reflection of the fact that scaling Q can be offset by scaling P and m or ω when the Hamiltonian is cyclic. The generating function can also undergo arbitrary translations of the Q variable as well, which are offset simply by choosing a different value for Q_i in the classical solution.

The classical harmonic oscillator solution can be generalized to power potentials of the form

$$H = \frac{p^2}{2m} + \frac{1}{n}m\lambda^n q^n\,, \tag{53}$$

where λ is a constant with the natural units of inverse length. Hamiltonians of the form (53) are rendered cyclic by using the generating function

$$F = -\frac{1}{2\alpha}\left(\frac{p^2}{m\lambda}\right)^\alpha f^\gamma(Q)\,, \tag{54}$$

where $\alpha = (n+2)/2n$ and $\gamma = -2/n$. Using this generating function gives

$$q = \frac{p^{2\alpha-1}}{(m\lambda)^\alpha} f^\gamma(Q)\,, \tag{55}$$

$$P = \frac{\gamma}{2\alpha}\frac{p^{2\alpha}}{(m\lambda)^\alpha} f^{(\gamma-1)}(Q)\frac{\partial f(Q)}{\partial Q}\,. \tag{56}$$

Substituting (55) into the original Hamiltonian gives

$$H = p^2\left[\frac{1}{2m} + \frac{1}{n\lambda}\left(\frac{\lambda}{m}\right)^{\frac{n}{2}} f^{\gamma n}(Q)\right]\,. \tag{57}$$

Using (56) shows that (57) reduces to

$$\tilde{H} = \omega P^\beta\,, \tag{58}$$

where $\beta = 2n/(n+2) = 1/\alpha$, if $f(Q)$ is chosen to satisfy the first-order differential equation

$$\frac{\partial f(Q)}{\partial Q} = \frac{2\alpha}{\gamma}\left(\frac{\lambda}{2\omega}\right)^\alpha \left[f^2(Q) + \frac{2m}{n\lambda}\left(\frac{\lambda}{m}\right)^{\frac{n}{2}}\right]^\alpha\,. \tag{59}$$

While a particular value for the ω in (58) can be chosen, such a choice is arbitrary in the same way that the ω' in (52) is arbitrary. This arbitrariness in scale is similar to that which appears in equivariant cohomology approaches to the same problem [18]. The sign for ω is determined from the range of the original Hamiltonian, and can be either positive or negative if the original Hamiltonian was such that $n < 0$. Choosing a negative sign for ω will affect the final form of expression (59). However, it is important to note that if n is odd, the range of the original Hamiltonian is $-\infty$ to ∞. This will introduce difficulties in maintaining the range of the Hamiltonian in some cases. This will be demonstrated for the specific case of a linear potential in Sec. V B.

Equation (59) can be formally solved by integration, so that

$$\frac{2\alpha}{\gamma}\left(\frac{\lambda}{2\omega}\right)^\alpha (Q - Q_i) = \int \frac{df}{[f^2+\zeta^2]^\alpha}\,, \tag{60}$$

where

$$\zeta^2 = \frac{2m}{n\lambda}\left(\frac{\lambda}{m}\right)^{\frac{n}{2}}\,. \tag{61}$$

The right-hand side of (60) is, up to the factor on the left-hand side, the functional inverse of f, written g, so that $g(f(Q)) = Q$. Therefore, inverting (60), where possible, yields the function $f(Q)$ appearing in the canonical transformation. However, even if the expression generated by (60) cannot be exactly inverted, it can still be used to determined the classical form for $Q(q,p)$ in the following way. Form (55) shows that

$$Q = g\left(\left[\frac{m^\alpha\lambda^\alpha q}{p^{2\alpha-1}}\right]^{\frac{1}{\gamma}}\right)\,, \tag{62}$$

so that the result of the integral (60), written as a function of f, must coincide with result (62). Therefore substituting

$$f = \left(\frac{m^{\alpha}\lambda^{\alpha}q}{p^{2\alpha-1}}\right)^{\frac{1}{\gamma}} \tag{63}$$

into the result of the integration in (60) gives $Q = Q(q,p)$. It is easy to show that the choices $n = 2$, $\omega = \lambda$, and $Q_i = \pi/2$ reproduce the harmonic oscillator generating function (52). However, the cyclic form (58) for the transformed Hamiltonian is not unique since a second transformation using the generating function $F = -f(P)Q'$ results in a Hamiltonian that is an arbitrary function of $P' = f(P)$ alone. Nevertheless, in any cyclic Hamiltonian the remaining variable is some function of the original Hamiltonian, i.e., $P = P(H(p,q))$.

Any attempts to use these results within the quantum-mechanical context are immediately beset with ordering problems. While the classical Poisson bracket of Q and P remains unity, the original algebra of q and p, coupled with the transcendental nature of the transformation, results in the commutator of Q and P being poorly defined. To lowest order in $\hbar$ it is true that $[Q,P] = i\hbar$, but additional powers appear that are dependent on the ordering convention chosen for the expansion of the transcendental functions. In order to preserve the commutation relations it is necessary to institute a unitary transformation of the original operator variables, rather than a canonical transformation. Anderson [19] has discussed enlarging the Hilbert space of the original theory to accommodate nonunitary transformations that alter the commutation relations. Although some of the results obtained in such an approach are similar to those of canonical transformations, this is a fundamentally different approach to solving the equations of motion. As a result, it will not be discussed here.

These ordering ambiguities can be demonstrated by examining the canonical transformation from Cartesian to spherical coordinates in two dimensions. The generating function for this transformation is given by

$$F = -p_x r\cos\theta - p_y r\sin\theta\,, \tag{64}$$

and this yields the standard result $x = r\cos\theta$, $y = r\sin\theta$, $P_r = p_x\cos\theta + p_y\sin\theta$, and $P_\theta = -p_x r\sin\theta + p_y r\cos\theta$. In order to invert these equations it is necessary to choose an ordering convention for the operators. The most reliable of these is Weyl ordering, which symmetrizes all noncommuting operators. The result is

$$p_x = \cos\theta\,P_r - \frac{\sin\theta}{2r}P_\theta - P_\theta\frac{\sin\theta}{2r}\,, \tag{65}$$

$$p_y = \sin\theta\,P_r + \frac{\cos\theta}{2r}P_\theta + P_\theta\frac{\cos\theta}{2r}\,. \tag{66}$$

Using the commutators for the spherical coordinates yields

$$p_x^2 + p_y^2 = P_r^2 + \frac{1}{r^2}P_\theta^2 + \frac{i\hbar}{r}P_r - \frac{\hbar^2}{4r^2}\,, \tag{67}$$

showing that this transformation takes a cyclic Hamiltonian into a noncyclic Hamiltonian. It is not difficult to see that the $O(\hbar)$ term is essential to maintaining self-adjointness of the Hamiltonian when written in terms of spherical coordinates. This can be seen from an integration by parts for the expectation value of the Hamiltonian in spherical coordinates [16]. Of course, such a term is not generated by the classical transformation, giving further evidence that classical canonical transformations and their quantum counterparts may differ by terms that are functions of $\hbar$. The numerical factor appearing before the $O(\hbar^2)$ term in (67) is a function of the Weyl ordering chosen for the original operator expressions.

Nevertheless, because $[Q,P] \approx i\hbar$, it is interesting to treat the new variables as if they were canonically conjugate quantum variables and pursue the solution of the transformed system (58). Alternatively, one could start with the Hamiltonian (58), enforce the exact commutator $[Q,P] = i\hbar$, and solve for the energy levels of the system. While it is clear that the previously mentioned ordering problems prevent this solution from being that of the original system that led to the cyclic Hamiltonian, such a solution can serve as an approximation to $O(\hbar^2)$ of the original Hamiltonian. It should be noted that there are many values for n such that the corresponding quantum theory is not well defined. For example, odd values of n correspond to unstable theories if the range of q is $[-\infty,\infty]$. Negative values of n are associated with pathologies; for example, the exponent β appearing in (58) diverges at $n = -2$. It will be assumed that the formal solution to be discussed is restricted to a theory that is well defined.

This solution can be found in a formal manner by assuming a discrete spectrum, i.e., bounded from below, and defining the creation and annihilation operators

$$a^\dagger = e^{iQ\hbar^{\alpha-1}}\sqrt{(P-\delta)\hbar^{-\alpha}}\,,\; a = \sqrt{(P-\delta)\hbar^{-\alpha}}\,e^{-iQ\hbar^{\alpha-1}}\,. \tag{68}$$

Using the commutator $[Q,P] = i\hbar$ gives $[a,a^\dagger] = 1$ regardless of the value of δ. Since $\hbar^\alpha a^\dagger a = P - (1+\delta)\hbar^\alpha$, the Hamiltonian (58) becomes $H = \hbar\omega(a^\dagger a + 1 + \delta)^\beta$. Defining a ground state $|\,0\,\rangle$ by the relation $a|\,0\,\rangle = 0$, it follows that the excitations of the system are obtained by applying suitably normalized factors of $a^\dagger$ to the ground state, leading to an energy spectrum $E_n = \hbar\omega(n+1+\delta)^\beta$.

The arbitrariness of δ can be used to offset the ordering ambiguities in the canonical transformation generated by the original algebra of q and p. The simple harmonic oscillator solution demonstrates this aspect. Using (51) and ignoring commutators of q and p shows that the annihilation operator of (68) contains the factor

$$e^{-iQ} = -i\sqrt{\frac{m\omega}{2P}}\left(q + \frac{ip}{m\omega}\right)\,. \tag{69}$$

The term in parentheses in (69) is, up to a factor, the standard annihilation operator associated with the harmonic oscillator. It is also true that ignoring the ordering ambiguities has resulted in an expression that does not satisfy $e^{-iQ}e^{iQ} = 1$ at the quantum level, exposing the formal nature of the manipulations that led to (69).

Choosing $\delta = -1/2$ reproduces the correct harmonic oscillator energy spectrum.

It is important to determine if the general form for the bound state spectrum of the Hamiltonian is in any way valid for other systems, since the harmonic oscillator is a notoriously pliable system. Choosing $n = -1$ in (53) and restricting to $\lambda, q > 0$ produces the one-dimensional Coulomb potential, whose associated Schrödinger equation can be readily solved by standard methods. The eigenvalue equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dq^2} - \frac{m}{\lambda q}\right)\psi_n(q) = E_n\psi_n(q) \tag{70}$$

possesses the bound state energies $E_n = -m^3/(2\hbar^2\lambda^2 n^2)$. The canonically transformed Hamiltonian (53) gives $\beta = -2$ for this case, so that the choice $\omega = -m^3/(2\hbar^3\lambda^2)$ and $\delta = 0$ reproduces the bound state energy spectrum of the Schrödinger equation since $\tilde{H} = -\hbar|\omega|(a^\dagger a + 1)^{-2}$. In addition, it is possible to evaluate the integral (60) for this case. Following the prescription outlined in (62) and (63) and using the value ω determined from the differential equation gives the result

$$\hbar^{3/2}(Q - Q_i) = -\left(\frac{\lambda^2}{2m^3}\right)^{\frac{1}{2}} pq\sqrt{\frac{m}{\lambda q} - \frac{p^2}{2m}} -2\arcsin\sqrt{\frac{\lambda q p^2}{2m^2}}\,. \tag{71}$$

The associated annihilation operator (68) possesses the factor

$$\begin{aligned}\exp(-iQ\hbar^{-3/2}) &\propto \exp\left(2i\arcsin\sqrt{\frac{\lambda q p^2}{2m^2}}\right) \\ &= -\frac{2\lambda q}{m}\left(H(p,q) + \frac{m}{2\lambda q}\right) \\ &\quad +2i\sqrt{-\frac{\lambda^2 q^2 p^2}{2m^3}H(p,q)}\,. \end{aligned} \tag{72}$$

Setting the Hamiltonian equal to its ground state eigenvalue, $E_1 = -m^3/(2\lambda^2\hbar^2)$, reduces (72) to

$$a \propto \frac{m^2}{\lambda\hbar^2}q - 1 + \frac{i}{\hbar}qp \to \frac{m^2}{\lambda\hbar^2}q - 1 + q\frac{\partial}{\partial q}\,, \tag{73}$$

and this differential operator annihilates the ground state wave function determined from the Schrödinger equation, $\psi_0 = Cq\exp(-m^2 q/\hbar^2\lambda)$.

As another example, letting $n \to \infty$ in (53) produces a potential that is zero for $|q| < 1/\lambda$ and infinite for $|q| > 1/\lambda$. This limit therefore corresponds to a particle in an infinite well of width $2/\lambda$. In this limit $\beta \to 2$, so that choosing $\omega = \pi^2\lambda^2\hbar/8m$ and $\delta = -1$ allows (58) to reproduce the standard square well energy spectrum $E_n = n^2\hbar\omega$. The form for $f(Q)$ given by (60) for this limit is not useful since it can be shown to correspond to a mapping of the interval $2/\lambda$ into the whole real line.

It is, however, possible to solve the classical square well problem using a canonical transformation of the form $F(p, Q) = -p\,f(Q)$, where the function f is chosen to be

$$f(Q) = \frac{8}{\lambda\pi^2}\sum_{n=1,3,5,\ldots}^{\infty}\frac{(-1)^{(n-1)/2}}{n^2}\sin(n\pi Q)\,. \tag{74}$$

The Fourier series (74) is the sawtooth wave with unit period and maxima and minima of $\pm\lambda^{-1}$. The derivative of (74) gives the square wave with values $\pm 2\lambda^{-1}$, so that

$$\left(\frac{\partial f(Q)}{\partial Q}\right)^2 = \frac{4}{\lambda^2}\,. \tag{75}$$

As a result, the free Hamiltonian is mapped into another free Hamiltonian under the action of the canonical transformation,

$$P = p\,\frac{\partial f(Q)}{\partial Q} \Rightarrow \frac{p^2}{2m} \to \frac{\lambda^2 P^2}{8m}\,, \tag{76}$$

so that the classical result for the evolution of Q is

$$Q = Q_i + \frac{\lambda^2 Pt}{4m}\,. \tag{77}$$

Whereas the original momentum p oscillates between a positive and negative value, the new variable P is truly a constant of motion. The classical canonical transformation gives

$$q = f\left(Q_i + \frac{\lambda^2 Pt}{4m}\right)\,,\quad p = \frac{P}{\frac{\partial f}{\partial Q}}\,, \tag{78}$$

and this describes the bouncing motion of the classical particle in the square well.

IV. QUANTUM CANONICAL TRANSFORMATIONS AND ANOMALIES

In the operator approach to quantum-mechanical systems any nontrivial change of variables is complicated by the ordering and noncommutativity of the constituent operators that occur in expressions. Such difficulties are not immediately apparent in the path-integral expression (7) due to the c-number form of the variables in the action. However, closer inspection of the action in (7) shows that the formal time derivatives do not behave in a way that allows the classical canonical transformation to be implemented, since $q_{j+1} - q_j$ is not *a priori* $O(\epsilon)$. For this reason the implementation of canonical transformations in the path-integral formalism cannot in general reproduce the transformed classical action. In fact, it would be an error in most cases if it did, since using the classical result in the action of the transformed path integral would yield a transition element that was inconsistent with the results obtained from the Schrödinger equation, operator techniques, or the original untransformed path integral. An alternate approach must be taken, and in this paper a variant of the method of Fukutaka and Kashiwa [15] will be used. This approach can be inferred by examining the ramifications of using a new set of canonically conjugate variables to construct the path integral.

The phase space of a quantum-mechanical system may possess unusual properties, as the following simple argument demonstrates. The standard configuration space transition element can be written

$$\langle q(0) \mid q(T), T \rangle = G(q(0), q(T), T) \exp iW(q(0), q(T), T), \tag{79}$$

and upon taking the modulus squared, integrating over $q(T)$, and using the completeness of the position states, it follows that

$$\int dq(T)\, |G(q(0), q(T), T)|^2 = \langle q(0) \mid q(0) \rangle = \int \frac{dp(0)}{2\pi\hbar}\,. \tag{80}$$

For a quadratic Hamiltonian, it is well known that the function G is independent of $q(0)$ and $q(T)$ [1], so that (80) relates the volumes of quantum phase space components to each other. For example, the free particle is such that

$$G(q(0), q(T), T) = \sqrt{\frac{m}{2\pi i\hbar T}}\,, \tag{81}$$

so that (80) gives

$$\int dq(T) = \frac{T}{m} \int dp(0)\,. \tag{82}$$

Result (82) is reminiscent of the spreading of a wave packet for the free particle. A similar analysis for the harmonic oscillator gives

$$\int dq(T) = \frac{\sin \omega T}{m\omega} \int dp(0)\,. \tag{83}$$

Of course, both of the phase space volumes appearing in these expressions are infinite, and the comparison of infinities is a poorly defined endeavor. Nevertheless, these results hint at a richer structure in the quantum-mechanical phase space, and that this structure is related to the prefactor G.

If there exist new conjugate operators, $\hat{Q}$ and $\hat{P}$, at the quantum level, it is then natural to construct the path integral using their eigenstates as intermediate states. This means a repetition of the steps used in Sec. II that led to (7), using as a unit projection operator

$$\hat{1} = \int \frac{dP}{\sqrt{2\pi\hbar}}\, dQ \mid Q \rangle e^{iQP/\hbar} \langle P \mid. \tag{84}$$

In so doing, two difficulties occur immediately. The first is the evaluation of the matrix elements of the original Hamiltonian, $H(\hat{p}, \hat{q}, t)$, in the new states. The second problem is the end point evaluation. While the intermediate states are the new ones, the end point states of the transition element are still eigenstates of the old operators. In the transition element of (1) there are two inner products of importance to the final form of the path integral constructed using N copies of the unit projection operator (84), and these are $\langle p_f \mid Q_N \rangle$ and $\langle P_1 \mid q_i \rangle$. In some simple cases, such as the transformation from Cartesian to polar coordinates, it is possible to obtain exact expressions for these inner products. In most cases it is not. In order to evaluate these inner products, a general form for them will be assumed, and a consistency condition necessary to maintain (84) as a unit projection operator will be derived. This result will serve to define a quantum-mechanical version of canonical transformations that is similar in structure to that proposed by Fukutaka and Kashiwa [15].

If (84) is to hold, the form of the inner products must be such that

$$\langle p_f \mid q_i \rangle = \int \frac{dP_1}{\sqrt{2\pi\hbar}}\, dQ_N \langle p_f \mid Q_N \rangle e^{iP_1 Q_N/\hbar} \langle P_1 \mid q_i \rangle\,. \tag{85}$$

The new variables and the inner products are defined in the following way. The inner products are written formally in terms of some function $F(p, Q)$,

$$\langle p_f \mid Q_N \rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left\{\frac{i}{\hbar}\,[P_f(Q_f - Q_N) + F(p_f, Q_f)]\right\}, \tag{86}$$

$$\langle P_1 \mid q_i \rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left\{-\frac{i}{\hbar}\,[P_1 Q_i + F(p_i, Q_i)]\right\}. \tag{87}$$

Inserting forms (86) and (87) into (85) gives

$$\langle p_f \mid q_i \rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left\{\frac{i}{\hbar}\left[P_f(Q_f - Q_i) + F(p_f, Q_f) - F(p_i, Q_i)\right]\right\}. \tag{88}$$

In order that (88) reduce to the standard result, it is necessary to identify

$$-P_f(Q_f - Q_i) = F(p_f, Q_f) - F(p_f, Q_i)\,, \tag{89}$$

$$-q_i(p_f - p_i) = F(p_f, Q_i) - F(p_i, Q_i)\,. \tag{90}$$

For the identifications of (89) and (90) the inner product of (88) reduces to

$$\langle p_f \mid q_i \rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left[-\frac{i}{\hbar}\, q_i(p_f - p_i)\right], \tag{91}$$

which is the correct result if the restriction $p_i = 0$, familiar from the discussion in Sec. II B, is enforced.

Although identifications (89) and (90) result in infinite series definitions of the new variables P and Q, the leading term of the expansions reproduces the classical result. For example, (89) gives

$$P_f = -\frac{\partial F(p_f, Q_f)}{\partial Q_f} + \frac{1}{2}\frac{\partial^2 F(p_f, Q_f)}{\partial Q_f^2}(Q_f - Q_i) + \cdots, \tag{92}$$

so that the first term coincides with the time-independent form of the classical canonical transformation to the new variable P. In addition, the quantum counterparts of identities such as (47) are altered. This will be discussed later in this section.

The "infinitesimal" versions of (89) and (90), to be used in defining the path-integral variables, are given by

$$P_j = -\frac{F(p_j,Q_j)-F(p_j,Q_{j-1})}{\Delta Q_j}, \qquad (93)$$

$$q_j = -\frac{F(p_{j+1},Q_j)-F(p_j,Q_j)}{\Delta p_j}, \qquad (94)$$

where $\Delta Q_j = Q_j - Q_{j-1}$ and $\Delta p_j = p_{j+1} - p_j$. Using these definitions of the new variables allows the formal time derivatives in the path-integral action to be transformed appropriately, since (93) and (94) give

$$-q_j(p_{j+1}-p_j) = P_{j+1}(Q_{j+1}-Q_j) + F(p_{j+1},Q_{j+1}) - F(p_j,Q_j), \qquad (95)$$

and the action sum in the path-integral (7) therefore becomes

$$-\sum_{j=0}^{N} q_j(p_{j+1}-p_j) = F(p_f,Q_f) - F(p_i,Q_i) + \sum_{j=0}^{N} P_{j+1}(Q_{j+1}-Q_j). \qquad (96)$$

Result (96) is similar in form to the standard end point terms generated in the action by a canonical transformation. It is important to remember that this result is valid only for the case that $p_i = 0$.

The form of the transformed Hamiltonian appearing in the action is complicated by the dependence of the old variables, q and p, on ΔP and ΔQ, as well as P and Q. From (93) it follows that p_j is a function of P_j, Q_j, and Q_{j-1}, but that the dependence on Q_{j-1} can be expressed in a power series in ΔQ_j,

$$P_j = \sum_{n=1}^{\infty} \frac{1}{n!}\frac{\partial^n F}{\partial {Q_j}^n}(-\Delta Q_j)^{n-1}. \qquad (97)$$

The importance of the leading behavior of ΔQ in ϵ, discussed in Sec. II B, is now apparent. The form of the transformed Hamiltonian will depend critically on whether the terms containing ΔQ and ΔP are suppressed by the overall factor of ϵ that prefaces the Hamiltonian. It should be clear from the discussion of Sec. II that these Δ terms will be suppressed by *some* power of ϵ; it is not clear until the specific system and transformation are chosen if they will still contribute to the path integral when the infinite sum is evaluated. If they do, then the transformed quantum-mechanical Hamiltonian will differ from the classical transformed Hamiltonian. The transformed Hamiltonian will therefore be written $H(p_j,q_j) = \tilde{H}(P_j,Q_j,\Delta P_j,\Delta Q_j)$, since it is not *a priori* obvious that the Δ terms can be suppressed. From the discussion in Sec. II B it is apparent there are cases where such terms can contribute to the evaluation of the path-integral, and, at least for one of the cases discussed there, can become $O(\hbar)$ terms. These are the path integral counterparts of the ordering ambiguities in the operator approach to canonical transformations, and, in a loose sense, represent commutators between the old canonical variables $\hat{q}$ and $\hat{p}$.

These results can be generalized to the case that the function F or the original Hamiltonian have explicit time dependence. Denoting the function as $F(p_j,Q_j,t_j)$, an analysis similar to that which led to (93) and (94) gives

$$P_j = -\frac{F(p_j,Q_j,t_j)-F(p_j,Q_{j-1},t_j)}{\Delta Q_j}, \qquad (98)$$

$$q_j = -\frac{F(p_{j+1},Q_j,t_j)-F(p_j,Q_j,t_j)}{\Delta p_j}, \qquad (99)$$

$$H(p_j,q_j,t_j) = \tilde{H}(P_j,Q_j,\Delta Q_j,\Delta P_j,t_j) + \frac{\partial F(p_{j+1},Q_j,t_j)}{\partial t_j}. \qquad (100)$$

The result (100) is valid only in the limit that $t_{j+1}-t_j = \epsilon \to 0$. However, the identifications of (98)–(100) lead to a result similar to (96),

$$\sum_{j=0}^{N}[-q_j(p_{j+1}-p_j) - \epsilon H(p_j,q_j,t_j)] = F(p_f,Q_f,t_f) - F(p_i,Q_i,t_i) + \sum_{j=0}^{N}\left[P_{j+1}(Q_{j+1}-Q_j) - \epsilon\tilde{H}(P_j,Q_j,\Delta P_j,\Delta Q_j,t_j) - \epsilon\frac{\partial F(p_{j+1},Q_j,t_j)}{\partial t_j}\right]. \qquad (101)$$

However, it will now be shown that the Jacobian of a general transformation may contribute terms of $O(\Delta Q)$ and $O(\Delta P)$ to the action in such a way that they are not prefaced by a factor of ϵ. For that reason they cannot be ignored, since the sum in which they are embedded allows them to contribute a finite amount to the transformed action. These $O(\Delta Q)$ and $O(\Delta P)$ contributions are calculated from (94) and (95) using the implicit dependence of Q on q and p. Initially, these contributions will be calculated for the case of a one-dimensional system, and the generalization will be discussed afterward.

The starting point is the definition of the inverse Jacobian,

$$J^{-1} = \prod_{j=1}^{N}\left[\frac{\partial Q_j}{\partial q_j}\frac{\partial P_j}{\partial p_j} - \frac{\partial P_j}{\partial q_j}\frac{\partial Q_j}{\partial p_j}\right], \qquad (102)$$

where it has been assumed that Q_j and P_j depend primarily on q_j and p_j, i.e., that the dependence on the other variables is suppressed by some power of ϵ. It will be seen that this is a self-consistent assumption. The partial derivatives of P_j can be obtained to $O(\Delta Q)$ from the expansion (97) by using the implicit dependence of Q_j on q_j and p_j. The result is

$$\frac{\partial P_j}{\partial p_j} = -\frac{\partial^2 F}{\partial p_j \, \partial Q_j} - \frac{1}{2}\frac{\partial^2 F}{\partial Q_j^2}\frac{\partial Q_j}{\partial p_j} + \left[\frac{1}{2}\frac{\partial^3 F}{\partial p_j \, \partial Q_j^2} + \frac{1}{6}\frac{\partial^3 F}{\partial Q_j^3}\frac{\partial Q_j}{\partial q_j}\right]\Delta Q_j, \qquad (103)$$

$$\frac{\partial P_j}{\partial q_j} = -\frac{1}{2}\frac{\partial^2 F}{\partial Q_j^2}\frac{\partial Q_j}{\partial q_j} + \frac{1}{6}\frac{\partial^3 F}{\partial Q_j^3}\frac{\partial Q_j}{\partial q_j}\Delta Q_j \, . \qquad (104)$$

Direct substitution of (103) and (104) into (102) gives

$$J^{-1} = \prod_{j=1}^{N}\left[-\frac{\partial^2 F}{\partial p_j \, \partial Q_j}\frac{\partial Q_j}{\partial q_j} + \frac{1}{2}\frac{\partial^3 F}{\partial p_j \, \partial Q_j^2}\frac{\partial Q_j}{\partial q_j}\Delta Q_j\right] . \qquad (105)$$

Result (94) can now be differentiated and combined with the independence of q_j and p_j to obtain, to $O(\Delta p)$, the quantum counterpart of (47),

$$1 = \frac{\partial q_j}{\partial q_j} = -\frac{\partial^2 F}{\partial p_j \, \partial Q_j}\frac{\partial Q_j}{\partial q_j} - \frac{1}{2}\frac{\partial^3 F}{\partial p_j^2 \, \partial Q_j}\frac{\partial Q_j}{\partial q_j}\Delta p_j \, . \qquad (106)$$

The term Δp_j can be written in terms of an expansion in ΔQ_j and ΔP_j, so that to $O(\Delta)$

$$\Delta p_j = \frac{\partial p_j}{\partial Q_j}\Delta Q_j + \frac{\partial p_j}{\partial P_j}\Delta P_j \, . \qquad (107)$$

Combining (107) and (106) and inserting the result into (105) yields

$$J^{-1} = \prod_{j=1}^{N}\left[1 + \frac{1}{2}\left(\frac{\partial^3 F}{\partial p_j^2 \, \partial Q_j}\frac{\partial Q_j}{\partial q_j}\frac{\partial p_j}{\partial Q_j} + \frac{\partial^3 F}{\partial p_j \, \partial Q_j^2}\frac{\partial Q_j}{\partial q_j}\right) \times\Delta Q_j + \frac{1}{2}\frac{\partial^3 F}{\partial p_j^2 \, \partial Q_j}\frac{\partial Q_j}{\partial q_j}\frac{\partial p_j}{\partial P_j}\Delta P_j\right]. \qquad (108)$$

In general the lack of invariance for the measure of a path integral under a transformation, which itself is a symmetry of the action, is referred to as an anomaly [20]. In the case of (108), the anomaly arises due to the formal nature of time derivatives in the path-integral action, and has nothing to do with the behavior of the classical action under a canonical transformation. Nevertheless, (108) will be referred to as the anomaly and can be written, to lowest order, as

$$J^{-1} = \prod_{j=1}^{N}(1 + A_j \Delta Q_j + B_j \Delta P_j) \, , \qquad (109)$$

where

$$A_j = \frac{1}{2}\left(\frac{\partial^3 F}{\partial p_j^2 \, \partial Q_j}\frac{\partial Q_j}{\partial q_j}\frac{\partial p_j}{\partial Q_j} + \frac{\partial^3 F}{\partial p_j \, \partial Q_j^2}\frac{\partial Q_j}{\partial q_j}\right), \qquad (110)$$

$$B_j = \frac{1}{2}\frac{\partial^3 F}{\partial p_j^2 \, \partial Q_j}\frac{\partial Q_j}{\partial q_j}\frac{\partial p_j}{\partial P_j} \, . \qquad (111)$$

It is important to note that, even if ΔQ_j is $O(\epsilon)$, the cross terms in (109) can contribute finite quantities. This follows from the fact that

$$J^{-1} = \lim_{N\to\infty}\prod_{j=1}^{N}(1 + A_j \Delta Q_j + B_j \Delta P_j) = \lim_{N\to\infty}\exp\left[\sum_{j=1}^{N}\ln(1 + A_j \Delta Q_j + B_j \Delta P_j)\right] . \qquad (112)$$

As a result, the expansion of the logarithm creates terms of the form

$$J = \exp\left\{\frac{i}{\hbar}\sum_{j=1}^{N}[i\hbar A_j \Delta Q_j + i\hbar B_j \Delta P_j]\right\}, \qquad (113)$$

which can be absorbed into the transformed action of the path integral. It should be noted that these terms can contribute a finite quantity to the action even if ΔQ is $O(\epsilon)$ since $N\epsilon \to T$. For the same reason, if the Δ terms are $O(\epsilon)$ or smaller, then the higher powers in the expansion of the logarithm can be dropped. Because they are proportional to $\hbar$, terms of the form (113) are reminiscent of the velocity-dependent potentials (26) discussed in detail in Sec. II B. Clearly, if the Δ terms are not suppressed by a factor of ϵ, it will be necessary to retain higher-order terms in both the expansion of the Jacobian (102) as well as later in the expansion of the logarithm in (112).

These results may be generalized to the multidimensional case. The multidimensional versions of (93) and (94) are given by

$$-P_j^a \Delta Q_j^a = F(p_j^a, Q_j^a) - F(p_j^a, Q_{j-1}^a) \, , \qquad (114)$$

$$-q_j^a \Delta p_j^a = F(p_{j+1}^a, Q_j^a) - F(p_j^a, Q_j^a) \, , \qquad (115)$$

where a sum over the repeated index a is implicit. The definitions (114) and (115) do not yield a unique expression for each of the q_j^a and P_j^a since the Taylor series expansions can be separated in an arbitrary manner for each of the variables. In what follows, a symmetrized definition of each of the canonical variables will be used, so that

$$P_j^a = -\frac{\partial}{\partial Q_j^a}\sum_{n=0}^{\infty}\frac{(-1)^n}{(n+1)!}\frac{\partial^n F_j}{\partial Q_j^{a_1}\cdots\partial Q_j^{a_n}}\Delta Q_j^{a_1}\cdots\Delta Q_j^{a_n}, \qquad (116)$$

$$q_j^a = -\frac{\partial}{\partial p_j^a}\sum_{n=0}^{\infty}\frac{(-1)^n}{(n+1)!}\frac{\partial^n F_j}{\partial p_j^{a_1}\cdots\partial p_j^{a_n}}\Delta p_j^{a_1}\cdots\Delta p_j^{a_n}, \qquad (117)$$

where there is an implicit sum over any repeated pair of a_i coordinate indices. It is straightforward to repeat the analysis that led to (109) and (110) and this yields the multidimensional version of the anomaly to $O(\Delta)$,

$$J^{-1} = \prod_{j=1}^{N}(1 + A_j^a \Delta Q_j^a + B_j^a \Delta P_j^a) , \tag{118}$$

where

$$A_j^a = \frac{1}{2}\frac{\partial^3 F_j}{\partial p_j^b \partial p_j^c \partial Q_j^d}\frac{\partial p_j^b}{\partial Q_j^a}\frac{\partial Q_j^d}{\partial p_j^c} + \frac{1}{2}\frac{\partial^3 F_j}{\partial p_j^b \partial Q_j^c \partial Q_j^a}\frac{\partial Q_j^b}{\partial q_j^c} , \tag{119}$$

$$B_j^a = \frac{1}{2}\frac{\partial^3 F_j}{\partial p_j^b \partial p_j^c \partial Q_j^d}\frac{\partial p_j^b}{\partial P_j^a}\frac{\partial Q_j^d}{\partial q_j^c} . \tag{120}$$

Exponentiation of (118) leads to a result similar to (113).

The $O(\Delta)$ anomaly takes a particularly simple form when the original generating function is given, for the one-dimensional case, by

$$F = -p^\alpha f(Q) . \tag{121}$$

From the results of Sec. III it is clear that (121) is adequate to transform all arbitrary single power potentials to a cyclic form. The anomaly associated with (121) will be evaluated using the classical forms for the new variables. Such a procedure is consistent only to $O(\Delta)$. It follows that these classical forms are given by solving

$$q_j = \alpha (p_j)^{(\alpha-1)} f(Q_j) , \quad P_j = (p_j)^\alpha \frac{\partial f}{\partial Q_j} , \tag{122}$$

and these relations in turn show that

$$\frac{\partial Q_j}{\partial q_j} = \frac{1}{\alpha} p_j^{(1-\alpha)} \left(\frac{\partial f}{\partial Q_j}\right)^{-1} , \tag{123}$$

$$\frac{\partial p_j}{\partial Q_j} = -\frac{1}{\alpha} p_j \left(\frac{\partial f}{\partial Q_j}\right)^{-1} \frac{\partial^2 f}{\partial Q_j^2} . \tag{124}$$

Using (122)–(124) in (110) and (111) yields

$$A_j = -\frac{1}{2\alpha}\left(\frac{\partial f}{\partial Q_j}\right)^{-1}\frac{\partial^2 f}{\partial Q_j^2} , \tag{125}$$

$$B_j = \frac{1-\alpha}{2\alpha P_j} . \tag{126}$$

Similarly, using the multidimensional generating function

$$F = -p^a f^a(Q) \tag{127}$$

results in a vector anomaly solely of the A type, given by

$$A_j^a = -\frac{1}{2}\frac{\partial^2 f^b}{\partial Q_j^a \partial Q_j^c}\frac{\partial Q_j^c}{\partial q_j^b} . \tag{128}$$

It is important to note that if it is possible to treat $\Delta Q \approx \epsilon \dot{Q}$, then the exponentiated anomaly term of (125) becomes

$$-\lim_{N\to\infty}\sum_{j=1}^{N} A_j \Delta Q_j = -\int_0^T dt\, A(Q)\,\dot{Q} = \frac{1}{2\alpha}\int_0^T dt \frac{d}{dt}\ln\frac{\partial f(Q)}{\partial Q} . \tag{129}$$

For these conditions the entire A anomaly therefore reduces to a prefactor for the path integral, given by

$$A_p = \left(\frac{\partial f(Q_f)}{\partial Q_f}\right)^{1/2\alpha}\left(\frac{\partial f(Q_i)}{\partial Q_i}\right)^{-1/2\alpha} . \tag{130}$$

Similarly, the B anomaly can be written

$$-\lim_{N\to\infty}\sum_{j=1}^{N} B_j \Delta P_j = -\frac{1-\alpha}{2\alpha}\int_0^T dt \frac{\dot{P}}{P} = -\frac{1-\alpha}{2\alpha}\int_0^T dt \frac{d}{dt}\ln P . \tag{131}$$

As a result, the B anomaly creates a second prefactor,

$$B_p = \left(\frac{P_i}{P_f}\right)^{(1-\alpha)/2\alpha} . \tag{132}$$

Results (130) and (132) show that, even in the case that the canonically transformed Hamiltonian is cyclic and the transformed path integral generates no prefactor, it is still possible for the correct prefactor or van Vleck determinant to be recovered from the anomaly associated with the canonical transformation.

However, results (130) and (132) also show that the problem of identifying the appropriate boundary conditions for Q and P is of paramount importance to evaluating the anomaly and determining the correct prefactor for the original path integral. In previous sections it has been stressed that the use of a canonical transformation requires suppressing the p_i term that must be inserted into the action to allow the definition of the canonical transformation. On the face of it, simply setting p_i to zero would appear to be sufficient to bypass this problem. However, doing so would create three initial and final conditions for the classical system, thereby overspecifying the classical solution to the equations of motion, a solution that is critical to evaluating the path integral for cyclic coordinates. However, if q_i is set to zero, the p_i term is automatically suppressed since it appears in the action as $q_i p_i$. This choice therefore allows the value of p_i to be determined from the classical equations of motion consistent with the boundary conditions $q_i = 0$ and p_f arbitrary. The requirement that q_i, rather than p_f, be zero for consistency is an outgrowth of choosing to write the action with a term of the form $q\dot{p}$, rather than $p\dot{q}$. This in turn was a result of choosing a canonical transformation of the third kind. Other choices will lead to different consistency requirements.

In the case of quantized variables, the problem is yet more subtle. In Sec. II D the path integral with an action translated by a classical solution was evaluated and the fluctuation variables p_j and q_j, given by (37) and (38), were shown to be arbitrary at their undefined end point values, i.e., $q(t = T)$ and $p(t = 0)$. While this is a natural consequence of the uncertainty principle, it means that the original quantum variables do not collapse to their classical values at these times, i.e., $q(t = T) \neq q_c(t = T)$. Therefore using the classical definitions for both of the q and p end point values is not a reliable method. As in the classical case, if p_f is to be defined and p_i is to be arbitrary, i.e., nonzero, it is clear from the discussion in Sec. II B that the path integral must be evaluated at $q_i = 0$, since such a choice will suppress the p_i term while still allowing p_i to be arbitrary. The absence of q_f from the action of the path integral of the form (7) allows it to be arbitrary without encountering a similar problem. Thus the canonically transformed path integral's end point values are correct only if $q_i = 0$. For a canonical transformation of the form given by (121), this means that Q_i must be a root of $f(Q)$. This clearly also suppresses the initial value of the generating function $(p_i)^\alpha f(Q_i)$.

Obviously, the $q_i \neq 0$ case can be evaluated by first translating the action everywhere by the classical solutions, as in Sec. II D. This leaves a path integral with the effective boundary conditions $q_i = 0$ and $p_f = 0$, allowing a consistent evaluation. A drawback to this technique is that such a translation will create additional terms in the potential in most cases, and the simple canonical transformations introduced in Sec. III to render power potentials cyclic will no longer be applicable after the translation. However, if the original potential was linear or quadratic this will not be the case, since such a translation induces no additional terms in the fluctuation potential for these two cases. A translation by a classical solution then shows that the prefactor of the form (130) must be independent of the end point values for the case that the original potential was linear or quadratic, and should be evaluated consistent with the conditions $q_i = 0$ and $p_f = 0$.

Apart from these considerations, the transformed action with the anomaly term in it is given by

$$\sum_{j=1}^{N}[(P_j + i\hbar A_j)\Delta Q_j + i\hbar B_j \Delta P_j - \epsilon H(P_j, Q_j, \Delta Q_j, \Delta P_j)] \ . \quad (133)$$

If the range of the P_j integrations is $-\infty$ to $+\infty$, it is possible to move the anomaly into the Hamiltonian by translating the P_j variables to $P_j - i\hbar A_j$, so that the Hamiltonian becomes formally similar to that of a particle moving in a complex vector potential.

The anomaly appears because of the structure of quantum-mechanical phase space. The exact function of the anomaly depends on the specific system being evaluated. Some of these will be discussed in Sec. V.

V. EXAMPLES

In this section the machinery developed in the previous sections will be applied to specific cases to evaluate the path integral by a canonical transformation. In most of the cases the exact form of the path integral is available by other methods, so that the outcome of the canonical transformation may be compared to show that equivalent results are obtained.

A. Transformations of the free particle

In this subsection a specific set of canonical transformations of free particle systems will be considered. In Sec. II C the path integral (35) for the square well was derived. Through Poisson resummation it was shown to possess the same infinite range of integrations for the measure as that of a free particle. The path integral for the square well can therefore be evaluated by the techniques of (28) and (29) for cyclic Hamiltonians. This shows that the square well path integral reduces to the correct result, i.e., the value of the action along the classical trajectory with the additional overall factor of $1/\sqrt{2a}$. There is no need to perform a canonical transformation on this system.

However, since the exact solution of the free particle path integral is available, such a system can serve as a laboratory to investigate the validity of the techniques derived in previous sections. To begin with, the variables in the action will be translated by the classical solution to the equation of motion, so that the end point variables are given by $p_{N+1} = 0$ and $q_0 = 0$. Because it is quadratic in the momentum, the action is unaffected in form by this translation. However, the arguments of Sec. II C show that the remaining path integral should reduce to a factor of unity, even in the event that it is canonically transformed. In this subsection the effect of canonical transformations associated with the classical generating function $F = -p\, f(Q)$ on such a free particle path integral will be considered. Such a canonical transformation at the classical level creates a Hamiltonian that, for most choices of f, is velocity dependent. Such Hamiltonians are typically not self-adjoint, creating difficulties in constructing the Hilbert space of the theory. It is therefore of interest to examine how the transformed path integral sidesteps this problem.

This canonical transformation has the general form (121), so that, to $O(\Delta)$, the anomaly is given by

$$A_j = -\frac{1}{2}\left(\frac{\partial f}{\partial Q_j}\right)^{-1}\frac{\partial^2 f}{\partial Q_j^2} \ , \quad B_j = 0 \ . \quad (134)$$

It is important to investigate if the approximations used to derive (134) are valid, since the exact Jacobian may contain additional terms. The definitions of the new quantum-mechanical variables in (93) and (94) result in

$$q_j = f(Q_j), \quad (135)$$

$$p_j = \frac{P_j \Delta Q_j}{f(Q_j) - f(Q_{j-1})} = \left(\frac{\partial f(Q_j)}{\partial Q_j} - \frac{1}{2}\frac{\partial^2 f(Q_j)}{\partial Q_j^2}\Delta Q_j + \cdots\right)^{-1} P_j \ . \quad (136)$$

Because q_j is independent of P_j, the exact Jacobian for the jth product in the measure is given by

$$dp_j\,dq_j = dP_j\,dQ_j\,J_j$$
$$= dP_j\,dQ_j\left[1-\frac{1}{2}\left(\frac{\partial f(Q_j)}{\partial Q_j}\right)^{-1}\right.$$
$$\left.\times\frac{\partial^2 f(Q_j)}{\partial Q_j^2}\Delta Q_j+\cdots\right]^{-1}. \qquad (137)$$

When exponentiated, (137) yields the same $O(\Delta)$ result as (134).

However, it would be misleading to exponentiate this Jacobian for the following reason. The Hamiltonian in the path-integral action remains quadratic in momentum, since

$$\epsilon\frac{p_j^2}{2m} = \epsilon\frac{P_j{}^2}{2m}\left(\frac{\partial f}{\partial Q_j}\right)^{-2}$$
$$\times\left[1-\frac{1}{2}\left(\frac{\partial f(Q_j)}{\partial Q_j}\right)^{-1}\frac{\partial^2 f(Q_j)}{\partial Q_j^2}\Delta Q_j+\cdots\right]^{-2}. \qquad (138)$$

Even though the $O(\Delta Q)$ terms in the Hamiltonian could be treated as a perturbation, the presence of the ΔQ terms in the anomaly prevent integrating over the Q variables as in (28) to show that this remaining path integral reduces to unity. Instead, the P integrations must be performed first, and this shows that the anomaly in the measure is canceled as a result of the Gaussian P integrations. Since the action was translated by the classical solution *prior* to canonical transformation, the boundary conditions are $P_f = P_i = 0$ and $Q_f = Q_i = 0$. Upon performing the P integrations, the remaining Euclidean path integral reduces to

$$\int\prod_{i=1}^{N}\left[dQ_i\frac{\partial f(Q_i)}{\partial Q_i}\sqrt{\frac{1}{2\pi\hbar\epsilon}}\right]\exp\left\{-\frac{1}{\hbar}\sum_{j=1}^{N}\frac{m\Delta Q_j^2}{2\epsilon}\left(\frac{\partial f(Q_j)}{\partial Q_j}\right)^2\left[1-\frac{1}{2}\left(\frac{\partial f(Q_j)}{\partial Q_j}\right)^{-1}\frac{\partial^2 f(Q_j)}{\partial Q_j^2}\Delta Q_j+\cdots\right]^2\right\}. \qquad (139)$$

It is natural to define the new variables $f_j = f(Q_j)$, and this gives

$$df_i = dQ_i\frac{\partial f(Q_i)}{\partial Q_i}. \qquad (140)$$

This new variable must have the same range of integration as the original variable q_j by virtue of (135). The transformed action simplifies as well since

$$\frac{m\Delta Q_j^2}{2\epsilon}\left(\frac{\partial f(Q_j)}{\partial Q_j}\right)^2\left[1-\frac{1}{2}\left(\frac{\partial f(Q_j)}{\partial Q_j}\right)^{-1}\frac{\partial^2 f(Q_j)}{\partial Q_j^2}\Delta Q_j+\cdots\right]^2 = \frac{m\Delta Q_j^2}{2\epsilon}\left(\frac{\Delta f_j}{\Delta Q_j}\right)^2 = \frac{m\Delta f_j{}^2}{2\epsilon}. \qquad (141)$$

The resulting path integral is therefore identical to the original path integral written in terms of the q_j variables. The anomaly has been canceled by contributions from the Hamiltonian. This means that the path integral defined by the measure (137) and the action (138) maintains a well-defined quantum theory for a velocity-dependent Hamiltonian.

In general, it is not difficult to see that a canonical transformation resulting in a transformed Hamiltonian that is quadratic in P will possess $O(\Delta Q)$ terms that, upon integration of the P variables, can result in cancellation of the anomaly.

B. The linear potential

The case of the linear potential,

$$H = \frac{p^2}{2m} + m\lambda q\,, \qquad (142)$$

allows an exact integration of the path integral, yielding the transition element

$$W_{fi} = \frac{1}{\sqrt{2\pi\hbar}}\exp\left\{-\frac{i}{\hbar}\left[\frac{1}{2}T^2\lambda p_f + \frac{Tp_f^2}{2m} + q_i m\lambda T\right.\right.$$
$$\left.\left.+p_f q_i + \frac{1}{6}m\lambda^2T^3\right]\right\}. \qquad (143)$$

Since the action is linear, the effect of a canonical transformation on the path integral will be analyzed for the case that $p_f = q_i = 0$. Result (143) shows that the path integral with $p_f = q_i = 0$ must result in

$$W_{fi} = \frac{1}{\sqrt{2\pi\hbar}}\exp\left\{-\frac{i}{\hbar}\frac{1}{6}m\lambda^2T^3\right\}. \qquad (144)$$

The evaluation of this path integral by canonical transformation can be used as another test of the techniques developed in the previous sections. The classical action has the form (53) and can be rendered cyclic by a canonical transformation of the type (54). Evaluating the integral (60) for the classical generating function yields

$$F(p,Q) = -\frac{p^3}{6m^2\lambda}\left[\frac{8}{9m\lambda^2 Q^2} - 1\right] . \qquad (145)$$

However, this generating function suffers from a defect inherited from the parent Hamiltonian, which is not positive definite due to the odd power of q. Using the generating function of (145) yields the classical Hamiltonian

$$\tilde{H} = P^{2/3} , \qquad (146)$$

which is positive definite since P is assumed to range over real values and the real branch of the 2/3 power is used. In order to match the range of the original Hamiltonian, P would have to range over both pure real and pure imaginary values, rendering the integrations over P undefined. A similar problem exists for the range of the new canonical variable Q, since classically it is transformed to

$$Q^2 = \frac{8}{9m\lambda^2}\frac{p^2}{p^2 + 2m^2\lambda q} , \qquad (147)$$

resulting in imaginary values for the case that the original Hamiltonian is negative.

This problem can be remedied by adding the term $pE_0/m\lambda$ to the generating function (145), where the limit $E_0 \to \infty$ is understood. Doing so allows the range for P to be real while still matching the range of the original Hamiltonian, since the transformed Hamiltonian becomes

$$\tilde{H} = P^{2/3} - E_0 \;\Rightarrow\; P = \left(\frac{p^2}{2m} + m\lambda q + E_0\right)^{3/2} , \qquad (148)$$

while the range of Q is now real, since

$$Q^2 = \frac{8}{9m\lambda^2}\frac{p^2}{(p^2 + 2m^2\lambda q + 2mE_0)} . \qquad (149)$$

The necessary presence of E_0 stems from the fact that the Hamiltonian is not bounded from below.

Since the transformation does not yield a quadratic Hamiltonian, it will be assumed that the perturbative argument of Sec. II is valid, and that terms of $O(\Delta Q)$ in the transformed Hamiltonian can be suppressed. The transformed path integral is then given by

$$W_{fi} = \frac{A_p B_p}{\sqrt{2\pi\hbar}} \exp\left\{\frac{i}{\hbar}[F_f - F_i]\right\} \times \int \frac{dP}{2\pi\hbar}\, dQ \exp\left\{\frac{i}{\hbar}\int_0^T dt\,[P\dot{Q} - P^{2/3} + E_0]\right\} , \qquad (150)$$

where A_p and B_p are the anomaly prefactors (130) and (132), F_i and F_f are the generating function evaluated at the initial and final conditions, and all $O(\Delta Q)$ terms have been suppressed in the Hamiltonian.

Because the transformed Hamiltonian is cyclic, the results of Sec. II C show that the remaining path integral can be evaluated by finding the action along the classical trajectory. The initial and final conditions are determined from the equations of motion for the original variables, with the boundary conditions that p_f and q_i both vanish. The solutions for p and q consistent with these conditions are easily found, with the result that $p_i = m\lambda T$. Using (148) then gives

$$P_i = \left(\frac{1}{2}m\lambda^2 T^2 + E_0\right)^{3/2} , \qquad (151)$$

while

$$Q_i = \frac{2}{3}\sqrt{\frac{T^2}{E_0 - \frac{1}{2}m\lambda^2 T^2}} . \qquad (152)$$

The Hamiltonian equations of motion give

$$\dot{P} = 0 \;\Rightarrow\; P_f = P_i , \qquad (153)$$

$$\dot{Q} = \frac{2}{3}P^{-1/3} \;\Rightarrow\; Q_f = Q_i + \frac{2}{3}P_f{}^{-1/3}T . \qquad (154)$$

In the limit that $E_0 \to \infty$, it follows that $Q_f = Q_i$.

Using these results, the action along the classical trajectory becomes

$$\int_0^T dt\,[P\dot{Q} - P^{2/3} + E_0] = E_0 T - \int_0^T dt\,\frac{1}{3}P_i{}^{2/3} = \frac{2}{3}E_0 T - \frac{1}{6}m\lambda^2 T^3 . \qquad (155)$$

The generating functions reduce to

$$F_f = 0, \qquad (156)$$

$$F_i = \frac{2}{3}E_0 T . \qquad (157)$$

Finally, form (130) for the anomaly prefactor reduces to

$$A_p = \sqrt{\frac{Q_i}{Q_f}} \;\Rightarrow\; \lim_{E_0\to\infty} A_p = 1 , \qquad (158)$$

while the prefactor (132) becomes

$$B_p = \left(\frac{P_f}{P_i}\right)^{1/3} = 1 . \qquad (159)$$

Combining results (155)–(159) gives the correct result

$$\langle\, p_f = 0\,|e^{-iHT/\hbar}|\, q_i = 0\,\rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left\{-\frac{i}{\hbar}\frac{1}{6}m\lambda^2 T^3\right\} , \qquad (160)$$

showing that all reference to E_0 has disappeared from the problem. It is not difficult to extend the same analysis to the case that $q_i = 0$ and $p_f \neq 0$ to show that the correct results follow from the canonical transformation.

C. Polar coordinates

The transformation from Cartesian to polar coordinates served as the first indication that adopting classical canonical transformations to the path integral was more complicated than expected [9]. In effect, it is a multidimensional version of the transformation to a velocity-dependent potential analyzed in Sec. V A. As a result, a mechanism similar to (141) should occur, allowing the canonically transformed path integral to maintain its equivalence to the original path integral.

The starting point is the two-dimensional Hamiltonian

$$H = \frac{1}{2m}(p_x^2 + p_y^2) \; . \tag{161}$$

The action associated with this Hamiltonian may be transformed into polar coordinates by using the classical generating function

$$F = -p_x r \cos\theta - p_y r \sin\theta \; . \tag{162}$$

Of course, the quantum-mechanical version of this transformation results in terms of $O(\Delta)$ and higher. In the following analysis, the $O(\Delta)$ terms will be retained to construct the form of the path integral under this transformation. It is to be remembered throughout that this is a shorthand for the full canonical transformation. For simplicity, the boundary conditions will match those for the case that the original Cartesian action has been translated by the classical solutions to the equations of motion, so that $p_{xf} = p_{yf} = x_i = y_i = 0$. For such a choice the remaining path integral must reduce to a factor of unity.

The procedure is tedious but straightforward. The new momenta and coordinates are given by

$$\begin{aligned} P_{rj} = p_{xj}\left(\cos\theta_j + \frac{1}{2}\sin\theta_j\,\Delta\theta_j\right) \\ +p_{yj}\left(\sin\theta_j - \frac{1}{2}\cos\theta_j\,\Delta\theta_j\right) \; , \end{aligned} \tag{163}$$

$$\begin{aligned} P_{\theta j} = -p_{xj}\left(r_j\sin\theta_j - \frac{1}{2}\sin\theta_j\,\Delta r_j - \frac{1}{2}r_j\cos\theta_j\,\Delta\theta_j\right) \\ +p_{yj}\left(r_j\cos\theta_j + \frac{1}{2}\cos\theta_j\,\Delta r_j - \frac{1}{2}r_j\sin\theta_j\,\Delta\theta_j\right) \; , \end{aligned} \tag{164}$$

$$x_j = r_j\cos\theta_j \; , \tag{165}$$

$$y_j = r_j\sin\theta_j \; . \tag{166}$$

These definitions yield p_x and p_y in terms of the new variables. Substituting them into the Hamiltonian gives the transformed Hamiltonian to $O(\Delta)$:

$$\tilde{H}_j = \frac{1}{2m}\left[P_{rj}^2 + \frac{1}{r_j^2}\left(1 - \frac{1}{2}\frac{\Delta r_j}{r_j}\right)^{-2} P_{\theta j}^2\right] \; . \tag{167}$$

Retention of the $O(\Delta)$ terms is essential since the transformed Hamiltonian (167) is not cyclic and also remains quadratic in the momenta. The anomaly term can be calculated to $O(\Delta)$ directly from the form of the transformations, or by using the multidimensional form (119). The resulting measure for the path-integral transforms according to

$$dx_j\,dy_j\,dp_{xj}\,dp_{yj} \to d\theta_j\,dr_j\,dP_{\theta j}\,dP_{rj}\left(1 - \frac{1}{2}\frac{\Delta r_j}{r_j}\right)^{-1} \; . \tag{168}$$

It is possible to exponentiate the anomaly, resulting in terms in the transformed action with the form

$$\left(P_{rj} - \frac{i\hbar}{2r_j}\right)\Delta r_j \; . \tag{169}$$

Since the range of the P_{rj} integrations is infinite, this extra term can be transferred to the Hamiltonian by translating the P_{rj} variables. This results in

$$\frac{1}{2m}P_{rj}^2 \to \frac{1}{2m}P_{rj}^2 + \frac{i\hbar}{2mr_j}P_{rj} - \frac{\hbar^2}{8mr_j^2} \; . \tag{170}$$

This is precisely the self-adjoint form (67) for the Weyl-ordered Hamiltonian in spherical coordinates discussed in Sec. III.

However, as in the case of the velocity-dependent transformation discussed in this section, it is misleading to exponentiate the anomaly term. This is demonstrated by performing the momentum integrations. The integration over P_θ exactly cancels the anomaly, and the resulting measure in the path integral is $r_j\,dr_j\,d\theta_j\,(2\pi/m\epsilon)$, while the action becomes

$$\sum_{j=1}^{N}\left[\frac{m}{2\epsilon}\Delta r_j^2 + \frac{m}{2\epsilon}r_j^2\left(1 - \frac{1}{2}\frac{\Delta r_j}{r_j}\right)^2\Delta\theta_j^2\right] \; . \tag{171}$$

Using (165) and (166) it is straightforward to show that (171) is, to $O(\Delta)$, the same as

$$\sum_{j=1}^{N}\left(\frac{m}{2\epsilon}\Delta x_j^2 + \frac{m}{2\epsilon}\Delta y_j^2\right) \; , \tag{172}$$

while the measure is the same as $dx_j\,dy_j(2\pi/m\epsilon)$. Thus the path integral with P_r and P_θ integrated generates a path integral and measure exactly equivalent to the original path integral with p_x and p_y integrated. Since the original path integral reduces to a factor of unity, this completes the proof that the path integral with its action constructed using (167) and measure given by (168) reduces to a factor of unity. This is an $O(\Delta)$ proof of equivalence, similar to the all order proof for the transformation to a velocity-dependent potential discussed in Sec. V A. This is in effect nothing more than a multidimensional version of the relationship (141), and could be extended to an all orders proof.

D. The harmonic oscillator

The harmonic oscillator has been analyzed by employing the canonical transformation (50)

$$F = -\frac{p^2}{2m\omega}\tan Q \; , \tag{173}$$

so that, in the nomenclature of Sec. III, $f(Q) = \tan Q/(2m\omega)$ and $\alpha = 2$. It will be reviewed here for the sake of completeness and because certain results will be used in Sec. V E. The results for the quantum version give

$$q_j = \frac{p_{j+1} + p_j}{2m\omega} \tan Q_j , \tag{174}$$

$$P_j \Delta Q_j = \frac{p_j^2}{2m\omega} (\tan Q_j - \tan Q_{j-1}) . \tag{175}$$

The classical canonical transformation leads to the transformed Hamiltonian $\tilde{H} = \omega P$. The quantum version of the transformation, given by (174) and (175), results in terms of $O(\Delta)$ in the transformed Hamiltonian. However, because the transformed Hamiltonian is not quadratic in P and is cyclic, it will be assumed that suppressing these terms is allowed by the perturbative argument of Sec. II B. A mild difference occurs since the range of the P variable is $[0, \infty]$. This prevents the transfer of the anomaly into the Hamiltonian. As a result, the anomaly terms will be evaluated using (130) and (132).

Performing the path integral using results (28) yields the transition element

$$W_{fi} = \frac{A_p B_p}{\sqrt{2\pi\hbar}} \exp\left\{ \frac{i}{\hbar} [F_f - F_i + S_{\rm cl}] \right\} , \tag{176}$$

where $S_{\rm cl}$ is the transformed action evaluated along a classical trajectory,

$$S_{\rm cl} = \int_0^T dt \left(P_c \dot{Q}_c - \omega P_c \right) . \tag{177}$$

Hamilton's equations of motion, $\dot{Q} = \omega$ and $\dot{P} = 0$, have the solutions $Q_f = Q_i + \omega T$ and $P_f = P_i$, showing that $S_{\rm cl} = 0$. The restriction to $q_i = 0$ is satisfied by the choice $Q_i = 0$. Using these results in (130) and (132) gives the anomalies

$$A_p = \left(\frac{\partial f(Q_f)}{\partial Q_f} \right)^{1/2\alpha} \left(\frac{\partial f(Q_i)}{\partial Q_i} \right)^{-1/2\alpha} = \frac{1}{\sqrt{\cos \omega T}} , \tag{178}$$

$$B_p = \left(\frac{P_i}{P_f} \right)^{(1-\alpha)/2\alpha} = 1 . \tag{179}$$

The product of the anomalies reproduces the correct prefactor (45). The generating functions become $F_i = 0$ and

$$F_f = -\frac{p_f^2}{2m\omega} \tan \omega T . \tag{180}$$

Comparison with (44) and (45) shows that combining these results in (176) yields the correct harmonic oscillator transition element for the case $q_i = 0$.

E. The time-dependent harmonic oscillator

One of the drawbacks to the techniques developed in this paper has been the restriction $q_i = 0$. Of course, it is possible to circumvent this problem by first translating the action by a classical solution to the equations of motion. The remaining path integral will then have the boundary condition $q_i = 0$ automatically. Unfortunately, for all but the quadratic and linear potentials, doing so induces additional terms into the action, preventing the use of the generating function (54) which was derived to render the simple power potential potential of (53) cyclic.

However, it is possible to treat any translated action with a potential involving terms higher than quadratic in first approximation as a time-dependent harmonic oscillator. This follows from the fact that the translated action will possess the form

$$\mathcal{L} = -q\dot{p} - \frac{p^2}{2m} - \frac{1}{2} \frac{\partial^2 V(q_c)}{\partial q_c^2} q^2 - \cdots , \tag{181}$$

where q_c is a classical solution to the original equations of motion consistent with the boundary conditions $q_c(t=0) = q_i$ and $p_c(t=T) = p_f$. The presence of a set of well-defined eigenvalues for the associated eigenvalue problem is of central importance in determining tunneling rates and stability of states in the quantum theory and is intimately related to Morse theory [21].

A canonical transformation approach to the remaining quadratic path integral, effectively a time-dependent harmonic oscillator with the boundary conditions $q_i = p_f = 0$, will be used to obtain an approximate evaluation. This begins by defining the time-dependent frequency $\omega(t)$ by

$$[\omega(t)]^2 = \frac{1}{m} \frac{\partial^2 V(q_c)}{\partial q_c^2} . \tag{182}$$

The right-hand side of (182) can be negative for a wide variety of circumstances. For example, the potential $V(q) = -\beta q^2 + \lambda q^4$ gives rise to negative values for ω^2 along any trajectory that passes through the range of values $q^2 < \beta/6\lambda$. As a result many trajectories will generate an imaginary value for ω for intervals of t.

The time-dependent canonical transformation to be used is given by

$$F = -\frac{p^2}{2m\omega(t)} \tan Q , \tag{183}$$

where the time-dependent frequency of (182) appears in (183). Suppressing all terms of $O(\Delta)$ and using result (100), the transformed Hamiltonian for this case is given by

$$\tilde{H} = \omega(t) P + \frac{P}{2\omega(t)} \frac{\partial \omega(t)}{\partial t} \sin 2Q . \tag{184}$$

Clearly, suppressing the $O(\Delta)$ terms is not valid in this case since the transformed Hamiltonian is no longer cyclic. As a result, the analysis that follows must be considered as an attempt at an approximate but nonperturbative evaluation of the path integral. Hamilton's equations of motion are given by

$$\dot{Q} = \omega(t) + \frac{\partial \omega(t)}{\partial t} \frac{\sin 2Q}{2\omega(t)} , \tag{185}$$

$$\dot{P} = -\frac{\partial \omega(t)}{\partial t} \frac{\cos 2Q}{\omega(t)} P . \tag{186}$$

The solution to (185) depends upon the form of $\omega(t)$, but in general it cannot be formally expressed as an integral. The exact solution can be obtained by first solving the associated equation

$$\frac{d^2\psi}{dt^2} = -\left(\omega^2 - \frac{2\dot{\omega}^2}{\omega^2} + \frac{\ddot{\omega}}{\omega}\right)\psi . \tag{187}$$

The form for Q is then given by

$$Q(t) = \arctan\left(-\frac{\dot{\omega}\psi + \omega\dot{\psi}}{\omega^2\psi}\right) . \tag{188}$$

Once the form for $Q(t)$ is known, it is straightforward to solve (186) by formal integration to obtain

$$\frac{P_f}{P_i} = \exp\left\{-\int_0^T dt \left(\frac{\partial\omega(t)}{\partial t}\frac{\cos 2Q(t)}{\omega(t)}\right)\right\} . \tag{189}$$

The classical action along the trajectory given by (185) vanishes, while by virtue of the boundary conditions, $F_i = F_f = 0$. The entire translated path integral therefore reduces to the prefactor generated by the anomalies, and this is given by

$$\frac{1}{\sqrt{2\pi\hbar\cos Q(T)}}\exp\left\{-\int_0^T dt \left(\frac{\partial\omega(t)}{\partial t}\frac{\cos 2Q(t)}{4\omega(t)}\right)\right\} . \tag{190}$$

The exact form for the general time-dependent harmonic oscillator prefactor has been obtained by Lo [22]. Applying Lo's result to the specific case considered here gives the following time-dependent prefactor for the $q_i = p_f = 0$ transition element:

$$\frac{1}{\sqrt{2\pi\hbar}}\left(\frac{F(0)}{F(T)} + F(0)\dot{F}(T)\int_0^T \frac{d\tau}{F^2(\tau)}\right)^{-1/2} , \tag{191}$$

where F is a solution of the associated equation

$$\ddot{F} = -\omega^2(t)F . \tag{192}$$

Comparing the two forms of the prefactor, (190) and (191), is hampered because of the difficulty in simultaneously finding exact solutions to the two differential equations, (187) and (192), for all but the trivial case $\omega(t) = \omega_0$, where the two results can be seen to coincide. However, it is possible to compare the two results for the case that T is small and ω is a slowly varying function of time, so that second derivatives and products of derivatives of ω can be ignored. Assuming that $\omega(0) \neq 0$, an approximate solution to (192) is then given by

$$F(t) \approx \cos Q(t)\sqrt{\frac{\omega(0)}{\omega(t)}} , \tag{193}$$

where

$$Q(t) = \int_0^t d\tau\, \omega(\tau) . \tag{194}$$

Form (194) is also the approximate solution to (185) for small times. Placing (193) into (191) gives the prefactor

$$\left(2\pi\hbar\cos Q(T)\sqrt{\frac{\omega(T)}{\omega(0)}}\right)^{-1/2} . \tag{195}$$

This is the same result obtained from (190) by using (194) and the approximation $\cos 2Q(t) \approx 1$, so that

$$\exp\left(\int_0^T dt\,\frac{\dot{\omega}}{4\omega}\cos 2Q(t)\right) \approx \left(\frac{\omega(T)}{\omega(0)}\right)^{1/4} . \tag{196}$$

Result (190) is, of course, dependent on the original form of the interaction prior to translation as well as the values of p_f and q_i. This is because the functional form for $\omega(t)$ depends on the original form of the interaction and the boundary conditions of the trajectory through (182).

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