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Finite-Dimensional Path-Summation Formulation for Quantum Mechanics

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The phase-space path-summation formulation of quantum theory is reviewed. The relationships to classical mechanics, and the greater generality (as compared with the original configuration-space path-summation formulation of Feynman) are stressed. Then the formulation is extended so that one can express the transition amplitude, between states (belonging to an arbitrary basis) of a finite-dimensional quantum system (with arbitrary Hamiltonian), in path-summation form.

I. INTRODUCTION

Dirac[1] first emphasized that a relationship exists between a quantum-mechanics transition amplitude and the classical-mechanics action function.

Consider a quantum system which has a classical analog, with canonical operators[2] X, P, and Hamiltonian H. Write the transition amplitude as

$$\langle x_1 | \exp(-iHt/\hbar) | x_0 \rangle \equiv \exp[iS'(x_1, x_0; t)/\hbar]. \quad (1.1)$$

Dirac argued that the complex-valued function S' is analogous to the real-valued action function

$$S(x_1, x_0; t) \equiv \int_0^t L(x(x_1, x_0; t), \dot{x}(x_1, x_0; t))dt.$$

$[x(x_1, x_0; t)$ is the actual classical trajectory beginning at x_0 at time zero and ending at x_1 at time t. L is the classical Lagrangian.$]$ It can be proved[3] that

$$\lim_{\hbar\to 0} S' = S, \text{ if the limit is real.} \quad (1.2)$$

This interesting manifestation[4] of the classical limit is not obtained for all Hamiltonians, because the limit is not necessarily real. For example, a Hamiltonian which is an odd function of p (and does not depend upon x) leads to a real transition amplitude (1.1):

$$\exp(iS'/\hbar) = (\pi\hbar)^{-1}\int_0^\infty dp \cos\{\hbar^{-1}[p(x_1 - x_0) - H(p)t]\},$$

so the real part of S' is just 0 or π in this case.

An important class of Hamiltonians that do satisfy (1.2), however, are the Hamiltonians of nonrelativistic classical mechanics for which (1.2) is the well-known lowest-order WKB approximation.

Dirac further showed the relevance of the classical principle of stationary action to quantum mechanics. Break the time interval t up into N intervals of duration ϵ ($t=N\epsilon$), and write $\exp(-itH/\hbar)$ as the product of N terms $\exp(-i\epsilon H/\hbar)$. Then it follows from (1.1) that

$$\exp\left[\frac{i}{\hbar}S'(x_N, x_0; t)\right]=\int dx_{N-1}\cdots dx_1 \exp\left\{\frac{i}{\hbar}[S'(x_N, x_{N-1};\epsilon)+\cdots+S'(x_r, x_{r-1};\epsilon)+\cdots+S'(x_1, x_0;\epsilon)]\right\} \tag{1.3}$$

If (1.2) is satisfied in the limit as $\hbar\to 0$, the exponent in (1.3) becomes the classical action, calculated for a continuous trajectory in configuration space. This trajectory passes through the points x_r at times $r\epsilon$, obeys the equations of motion in between these points, and suffers a discontinuity in velocity at these points. Dirac pointed out that in this limit, the major contribution to the integral in (1.3) will come from trajectories in the neighborhood of the actual classical trajectory for which the action is stationary.

Feynman[5] brought into consideration the limit of S' as $t\to 0$. His argument is limited to the class of nonrelativistic Hamiltonians quadratic in the velocity. For such Hamiltonians, one can show that S' is equal to S to first order in t (apart from an additive term that is independent of x_1, x_0). In other words, the classical action S "dominates" both the expansion of S' in powers of $\hbar$ and the expansion of S' in powers of t. Because of this, Feynman could prove that

$$\exp\left[\frac{i}{\hbar}S'(x, x_0;t)\right]=\lim_{\substack{\epsilon\to 0, N\to\infty\\ N\epsilon=t}}\int dx_{N-1}\cdots dx_1 \exp\left\{\frac{i}{\hbar}[S(x, x_{N-1};\epsilon)+\cdots+S(x_1, x_0;\epsilon)+Ni\hbar\tfrac{1}{2}\ln(2\pi i\hbar\epsilon/m)]\right\}, \tag{1.4}$$

i.e., S (plus an additive term) can be substituted for each S' in Eq. (1.3), because only terms up to first order in ϵ make a contribution to the transition amplitude when ϵ is sufficiently small.

Feynman's "path summation" expression (1.4) for the transition amplitude has a number of interesting features. First, a *real* function S determines the *complex* function S'. Second, S has the classical interpretation of the action. Third, following Dirac's argument, the classical limit $\hbar\to 0$ is manifest. In later work, Feynman as well as other authors[6] have tended to deemphasize these features. Equations such as (1.3) have been termed path-summation expressions, even though the exponent in the integrand may be complex and bear no relation to a classical action.

Unfortunately, Feynman's argument is restricted to a limited class of Hamiltonians, because usually S' is not equal to S to first order in t. Attempts[6-9] to extend this to other classes of Hamiltonians, or to the transition amplitude between eigenstates of operators other than the position operator, have met with only limited success. For this reason, one has not been able to regard the Feynman formulation as an alternative that is completely equivalent to quantum mechanics.

There is, however, a path-summation formulation based upon phase space, rather than configuration space, which holds the promise of being applicable to a wider class of Hamiltonians. It was first mentioned briefly by Feynman,[10] enlarged upon by Tobocman,[7] and later found independently by Davies,[11] and again by Garrod.[12] We shall review this phase-space formulation in the remainder of this introductory section, paralleling the discussion already given of the configuration-space formulation. Then we will present what appears to us to be a natural extension of this formulation to quantum systems with a finite number of degrees of freedom.

Consider the transition amplitudes

$$\langle p_1|\exp(-iHt/\hbar)|x_0\rangle\equiv(2\pi\hbar)^{-1/2}\exp[iS_1'(p_1, x_0;t)/\hbar], \tag{1.5a}$$

$$\langle x_1|\exp(-iHt/\hbar)|p_0\rangle\equiv(2\pi\hbar)^{-1/2}\exp[iS_2'(x_1, p_0;t)/\hbar]. \tag{1.5b}$$

The complex valued functions S_1', S_2' are analogous to the real valued functions:

$$S_1(p_1, x_0;t)\equiv S(x_1(p_1, x_0;t), x_0;t)-p_1x_1, \tag{1.6a}$$

$$S_2(x_1, p_0;t)\equiv S(x_1, x_0(x_1, p_0;t);t)+p_0x_0. \tag{1.6b}$$

S_1, S_2 are well-known classical generating functions of canonical transformations between x_0, p_0 and x_1, p_1. Indeed, one[3] can show that

$$\lim_{\hbar\to 0}S_1'=S_1, \tag{1.7a}$$

$$\lim_{\hbar\to 0}S_2'=S_2, \tag{1.7b}$$

where the limit is always real.[13]

Next, following Tobocman,[7] we break the time interval t up into $2N$ intervals of duration $\epsilon/2$, and write $\exp(-itH/\hbar)$ as the product of $2N$ terms $\exp(-i\epsilon H/2\hbar)$. Between pairs of terms we insert alternately the resolutions of the identity $\int dp|p\rangle\langle p|$ and $\int dx|x\rangle\langle x|$. Then it follows from (1.5) that

$$\exp\left[\frac{i}{\hbar}S'(x_{2N},x_0;t)\right]=(2\pi\hbar)^{-1}\int dp_{2N-1}\int dx_{2N-2}\cdots\int dx_2\int dp_1 \times\exp\left\{\frac{i}{\hbar}[S_2'(x_{2N},p_{2N-1};\tfrac{1}{2}\epsilon)+S_1'(p_{2N-1},x_{2N-2};\tfrac{1}{2}\epsilon)+\cdots+S_2'(x_2,p_1;\tfrac{1}{2}\epsilon)+S_1'(p_1,x_0;\tfrac{1}{2}\epsilon)]\right\}. \quad (1.8)$$

In the limit as $\hbar\to 0$, according to (1.6) and (1.7), the exponent in the integrand of (1.8) is just the classical action

$$S=\int[p\dot{x}-H(x,p)]dt \quad (1.9)$$

calculated for a certain *discontinuous* trajectory in phase space. This trajectory proceeds according to the classical equations of motion except for alternate discontinuities in position and momentum coordinates every $\frac{1}{2}\epsilon$ seconds.

There exists a classical variational principle[14] which states that the action integral (1.9) is stationary under arbitrary variations of *both* p and x, treated as independent variables, in the neighborhood of the actual classical trajectory in phase space. (The two Euler-Lagrange equations are just Hamilton's equations.) Thus, following Dirac's argument, in the limit $\hbar\to 0$ the major contribution to the integral in (1.8) comes from trajectories in the neighborhood of the actual classical trajectory, for which the exponent in the integrand is equal to the classical action and is stationary.

So far we have pointed out that Dirac's arguments involving configuration space have precise analogs in the context of phase space. We now turn to Feynman's path-summation expression, and consider its analog.

We might hope to pass from Eq. (1.8) to a path-summation expression by approximating S_2', S_2' in the exponent by their values to order ϵ, and taking the limit $\epsilon\to 0$. However, upon expanding (1.5) in powers of t, we find that to first order S_1', S_2' are not generally real:

$$S_1'(p_1,x_0;t)=-p_1x_0-t\langle p_1|H|x_0\rangle/\langle p_1|x_0\rangle+O(t^2), \quad (1.10a)$$

$$S_2'(x_2,p_1;t)=x_2p_1-t\langle x_2|H|p_1\rangle/\langle x_2|p_1\rangle+O(t^2). \quad (1.10b)$$

So substitution of (1.10) into (1.8) will not yield what we consider to be an acceptable path-summation expression. Suppose, however, that H is written in symmetrically ordered form:

$$H=\tfrac{1}{2}(A+A^\dagger), \quad A\equiv\sum_i c_iG_i(X)F_i(P) \quad (1.11)$$

(the constants c_i are real and will generally depend upon $\hbar$). We note that if $A^\dagger$ and A are substituted for H in (1.10a) and (1.10b), the resulting expressions will be real to first order in t. This suggests the following argument.

In analogy with (1.5) we define

$$\langle p_1|\exp(-itA^\dagger/\hbar)|x_0\rangle\equiv(2\pi\hbar)^{-1/2}\exp[i\tilde{S}_1(p_1,x_0;t)/\hbar], \quad (1.12a)$$

$$\langle x_2|\exp(-itA/\hbar)|p_1\rangle\equiv(2\pi\hbar)^{-1/2}\exp[i\tilde{S}_2(x_2,p_1;t)/\hbar]. \quad (1.12b)$$

To first order in t,

$$\tilde{S}_1=-p_1x_0-tH(x_1,p_0)+O(t^2), \quad (1.13a)$$

$$\tilde{S}_2=x_2p_1-tH(x_2,p_1)+O(t^2) \quad (1.13b)$$

[$H(x,p)$ is obtained from (1.11) by substituting the variables x,p for the operators X,P]. Equations (1.13) are the expressions for the classical generating functions S_1, S_2 [Eqs. (1.6)] to first order in t.

As (1.8) follows from (1.5), so it follows from (1.12) that

$$\langle x|[\exp(-i\epsilon A/2\hbar)\exp(-i\epsilon A^\dagger/2\hbar)]^N|x_0\rangle =(2\pi\hbar)^{-N}\int dp_{2N-1}\int dx_{2N-2}\cdots\int dx_2\int dp_1\exp\left\{\frac{i}{\hbar}[\tilde{S}_2(x,p_{2N-1};\tfrac{1}{2}\epsilon)+\tilde{S}_1(p_{2N-1},x_{2N-2};\tfrac{1}{2}\epsilon)+\cdots +\tilde{S}_2(x_2,p_1;\tfrac{1}{2}\epsilon)+\tilde{S}_1(p_1,x_0;\tfrac{1}{2}\epsilon)]\right\}. \quad (1.14)$$

We expect that the formal limit of (1.14), the phase-space path-summation expression

$$\exp\left[\frac{i}{\hbar}S'(x,x_0;t)\right] = \lim_{\substack{\epsilon\to 0,N\to\infty\\ N\epsilon=t}} (2\pi\hbar)^{-N}\int dp_{2N-1}\int dx_{2N-2}\cdots\int dx_2\int dp_1 \times\exp\left\{\frac{i}{\hbar}[S_2(x,p_{2N-1};\tfrac{1}{2}\epsilon)+S_1(p_{2N-1},x_{2N-2};\tfrac{1}{2}\epsilon)+\cdots+S_2(x_2,p_1;\tfrac{1}{2}\epsilon)+S_1(p_1,x_0;\tfrac{1}{2}\epsilon)]\right\} \tag{1.15}$$

can be rigorously justified for a wide class of Hamiltonians, as was done by Nelson[15] utilizing a theorem of Trotter[16] for the analogous Feynman expression (1.4).

Cohen[17] first showed that the path-summation expression (1.15) yields the transition amplitude generated by the symmetrized Hamiltonian operator (1.11). He also pointed out that different forms for $S(x,p;t)$ lead to transition amplitudes corresponding to differently ordered Hamiltonian operators, correcting an impression given by Kerner and Sutcliffe[18] that only one form for a phase-space path-integral formulation was possible (the form espoused by Garrod[12]). The realization that the phase-space formulation can be applicable to a wider class of Hamiltonians than is possible with the configuration-space formulation was implicit in the work of Davies,[11] but was first explicitly stated by Kerner and Sutcliffe[18] [however, a rigorous proof of (1.15) remains to be given].

In Secs. II and III of this paper, we shall show how to extend the path-summation formulation described here (i.e. corresponding to a symmetrized Hamiltonian) to finite-dimensional quantum systems. Our criterion for such an extension is the maintenance of as many features of the path-summation expression (1.15) as is possible. Thus we will not be able to relate the exponent in the path-summation expression to a classical action, or obtain a classical limit as $\hbar\to 0$, as such quantities do not exist for finite-dimensional quantum systems. However, we will demand that the path-summation exponent be real, we will require that equations [(1.11) through (1.15)] have finite dimensional analogs, and we will show (in Sec. IV) how the finite-dimensional path-summation expression reduces to (1.15) in the limit as the dimensionality becomes infinite.

II. FINITE-DIMENSIONAL QUANTUM SYSTEM

When one wishes to treat a finite-dimensional quantum mechanical system by a path-summation formulation, one must first answer the question: What is to be the nature of the "path?" In Feynman's path-integral formulation, the path may be regarded as an actual continuous classical trajectory in configuration space. However, since the coordinates of points in configuration space are also eigenvalues of the position operator, one may also regard the path as a "trajectory" through the possible eigenvalues. In fact, since it is actually only the eigenvalues at times $t=0,\epsilon,2\epsilon,\ldots,N\epsilon$ that are specified, one may visualize the physical system as "hopping" from eigenvalue to eigenvalue every ϵ seconds.

In the phase-space path-integral formulation, one could regard the physical system as tracing out a classical trajectory in phase space. But because the trajectory is discontinuous, much of the appeal to classical intuition is lost. We prefer to regard the system as proceeding along a "quantum mechanical trajectory," moving from one permitted eigenvalue to another (alternating between position eigenstate and momentum eigenstate). This latter point of view makes it possible to extend the phase-space path-summation formulation to finite-dimensional systems in a natural way.

Consider an n-dimensional quantum system with orthonormal basis vectors $|r\rangle(r=0,\ 1,\ldots,n-1)$, and Hamiltonian H. We wish to express the transition amplitude

$$\langle r|\exp(-iHt/\hbar)|r_0\rangle\equiv\exp[iS'(r,r_0;t)/\hbar] \tag{2.1}$$

in path-summation form. The $|r\rangle$ vectors may be regarded as the finite-dimensional analog of position eigenvectors. It is necessary to introduce another set of orthonormal basis vectors $|k\rangle(k=0,\ 1,\ldots,n-1)$, the finite-dimensional analog of momentum eigenvectors, which are defined by their projections on the $|r\rangle$ basis:

$$\langle r|k\rangle\equiv n^{-1/2}\exp(i2\pi rk/n)\,. \tag{2.2}$$

It is also useful to define operators R and K,

$$R|r\rangle=r|r\rangle\,,\quad K|k\rangle=k|k\rangle\,, \tag{2.3}$$

which we shall call "conjugate" operators, although they do not, of course, have the commutation relations enjoyed by X and P.

We saw in Sec. I that, while S',S_1',S_2' are not generally real (not even to first order in t), one may split the Hamiltonian into a sum of terms so that a path-integral form involving the real functions S,S_1,S_2 can be obtained. Accordingly, by analogy with (1.11) and (1.12), we define

$$\langle k|\exp(-itA^\dagger/\hbar)|r\rangle\equiv n^{-1/2}\exp[iS_1(k,r;t)/\hbar]\,, \tag{2.4a}$$

$$\langle r|\exp(-itA/\hbar)|k\rangle \equiv n^{-1/2}\exp[iS_2(r,k;t)/\hbar], \tag{2.4b}$$

where the operator A is restricted by the condition

$$H=\tfrac{1}{2}(A+A^{\dagger}) \tag{2.5}$$

and the further condition that S_1, S_2 be real to first order in ϵ. If these constraints are satisfied, then the following equation is correct *to order* ϵ:

$$\langle r|\exp(-i\epsilon H/\hbar)|s\rangle \approx \sum_{k=0}^{n-1}\langle r|\exp(-i\epsilon A/2\hbar)|k\rangle\langle k|\exp(-i\,\epsilon A^{\dagger}/2\hbar|s\rangle = n^{-1}\sum_{k=0}^{n-1}\exp\left\{\frac{i}{\hbar}[S_2(r,k;\tfrac{1}{2}\epsilon)+S_1(k,s;\tfrac{1}{2}\epsilon)]\right\}. \tag{2.6}$$

As a consequence of (2.6), we can express the transition amplitude in the path-summation form:

$$\langle r|\exp(-iHt/\hbar)|r_0\rangle = \lim_{\substack{\epsilon\to 0, N\to\infty\\ N\epsilon=t}} n^{-N}\sum_{k_{2N-1}}\sum_{r_{2N-2}}\cdots\sum_{r_2}\sum_{k_1}\exp\left\{\frac{i}{\hbar}[S_2(r,k_{2N-1};\tfrac{1}{2}\epsilon)+S_1(k_{2N-1},r_{2N-2};\tfrac{1}{2}\epsilon)+\cdots +S_2(r_2,k_1;\tfrac{1}{2}\epsilon)+S_1(k_1,r_0;\tfrac{1}{2}\epsilon)]\right\} \tag{2.7}$$

Equation (2.7), the finite-dimensional analog of (1.15), is rigorously correct. The limit in (2.7) exists, essentially because finite-dimensional matrices are bounded operators. S_1, S_2 need only be evaluated to order ϵ, and so are real.

To implement (2.7), we need to express S_1, S_2 in terms of matrix elements of H. This is accomplished as follows. The first term in the expansion of S_1, S_2 in powers of ϵ is found by setting $t=0$ in (2.4) and utilizing (2.2):

$$S_2(r,k;0)=-S_1(k,r;0)=2\pi\hbar rk/n. \tag{2.8}$$

By taking the complex conjugate of (2.4a) and comparing with (2.4b) we can express S_1 in terms of S_2:

$$S_2(r,k;\tfrac{1}{2}\epsilon)=-S_1(k,r;-\tfrac{1}{2}\epsilon)=\frac{2\pi\hbar}{n}rk-\tfrac{1}{2}\epsilon\langle r|a|k\rangle+O(\epsilon^2). \tag{2.9}$$

We have introduced an operator a with *real* matrix elements $\langle r|a|k\rangle$. [By expanding (2.4) in powers of t we find

$$\langle r|a|k\rangle \equiv \langle r|A|k\rangle/\langle r|k\rangle.] \tag{2.10}$$

Equation (2.9) is the analog of (1.13). In order that (2.6)

$$\langle r|\exp(-iH\epsilon/\hbar)|s\rangle \approx n^{-1}\sum_{k=0}^{n-1}\exp\left\{\frac{i}{\hbar}[2\pi\hbar k(r-s)/n-\tfrac{1}{2}\epsilon(\langle r|a|k\rangle+\langle s|a|k\rangle)]\right\} \tag{2.11}$$

hold to order ϵ, the matrix elements $\langle r|a|k\rangle$ must satisfy the equation

$$\langle r|H|s\rangle=(2n)^{-1}\sum_{k=0}^{n-1}[\langle r|a|k\rangle+\langle s|a|k\rangle]\exp[i2\pi k(r-s)/n] \tag{2.12}$$

The quantity in the exponent of (2.11) may be regarded as the finite-dimensional analog of the classical action (multiplied by $i\hbar^{-1}$, evaluated for ϵ seconds). In particular, $\frac{1}{2}[\langle r|a|k\rangle+\langle s|a|k\rangle]$ is the finite-dimensional analog of the classical Hamiltonian (averaged over ϵ seconds). $\langle r|a|k\rangle$ must be real and satisfy (2.12). We find (see Appendix) that

$$\langle r|a|k\rangle=\frac{2}{n}\sum_{k_1=0}^{n-1}\sum_{r_1=0}^{n-1}[1+\exp i\,2\pi k_1r_1/n]^{-1}\,\mathrm{Tr}[\exp(-i2\pi k_1(R-r)/n)H\exp(-i\,2\pi r_1(K-k)/n)] \tag{2.13}$$

is the solution of these constraints, *when it exists*.

Thus, given a finite-dimensional Hamiltonian operator H we can proceed to construct a path-summation expression for the transition amplitude as follows. First we use (2.13) to construct $\langle r|a|k\rangle$ (which is equivalent to finding the classical Hamiltonian in the infinite-dimensional problem). Then we use (2.9) to construct S_1, S_2 (which is equivalent to finding the classical action). Lastly we insert S_1, S_2 into the path-summation expression (2.7).

III. DISCUSSION

The solution for $\langle r|a|k\rangle$ certainly exists if the first term on the right-hand side of (2.13) is not infinite, i.e., if

$$\exp(i2\pi k_1 r_1/n) = -1 \quad (0 \le k_1, r_1 \le n-1) \tag{3.1}$$

is *not* satisfied. Satisfaction of (3.1) requires that

$$2k_1 r_1 = n(\text{odd integer}). \tag{3.2}$$

Clearly *the solution (2.13) exists for n odd,* since (3.2) cannot be fulfilled in this case.

When n is even there *are* certain values of r_1, k_1, for which (3.1) is satisfied. However, if the trace expression in (2.13) vanishes, then the solution for $\langle r|\,a\,|k\rangle$ exists (one omits these terms[19] from the sum). The vanishing of the trace expression implies the existence of linear relations between some matrix elements of H:

$$\sum_{s=0}^{n-1} \langle s|\exp(-i2\pi k_1 R/n) H \exp(-i2\pi r_1 K/n)|s\rangle = \sum_{s=0}^{n-1} \exp(-i2\pi k_1 s/n)\langle s|H|r_1+s\rangle = 0 \tag{3.3}$$

[in (3.3) we have employed the cyclic notation $|r+n\rangle \equiv |r\rangle$]. Sometimes the linear relations (3.3) can be satisfied, perhaps with an appropriate choice of the arbitrary phase factors multiplying the state vectors $|r\rangle$, perhaps with a reassignment of the numbers r to the eigenvectors.

We illustrate these equations by considering the case $n=2$. When $r_1 = k_1 = 1$, the condition (3.1) is satisfied, which tells us that the constraint equation (3.3) must be obeyed:

$$\langle 0|H|1\rangle - \langle 1|H|0\rangle = 0\,.$$

Since H is Hermitian, it is possible to satisfy this constraint by an appropriate choice of the phase factors of the states $|0\rangle$, $|1\rangle$. This makes the matrix $\langle r|H|s\rangle$ completely real; in fact, the matrix $\langle r|H|k\rangle$ is also real. We may then evaluate (2.13), obtaining

$$\langle r|\,a\,|k\rangle = \langle r|H|k\rangle / \langle r|k\rangle\,. \tag{3.4}$$

[From (3.4) and (2.10), it follows that $A=H$.] One may directly verify that (3.4) is indeed the solution of (2.12).

Incidentally, when $n=2$, Eq. (2.6) can be satisfied *exactly* (not merely to order ϵ) by an appropriate choice of S_2, S_1: This is not true for arbitrary n. Indeed, the most general 2×2 unitary matrix,

$$\exp i\varphi \begin{bmatrix} \cos\theta\exp(i\theta_1) & \sin\theta\exp(i\theta_2) \\ -\sin\theta\exp(-i\theta_2) & \cos\theta\exp(-i\theta_1) \end{bmatrix},$$

can be written in path-summation form

$$\tfrac{1}{2}\exp i\varphi \begin{bmatrix} \exp[-\tfrac{1}{2}i(\theta-\theta_1)] & i\exp[\tfrac{1}{2}i(2\theta_2+\theta+\theta_1)] \\ -i\exp[-\tfrac{1}{2}i(2\theta_2+\theta+\theta_1)] & -\exp[\tfrac{1}{2}i(\theta-\theta_1)] \end{bmatrix} \begin{bmatrix} \exp[-\tfrac{1}{2}i(\theta-\theta_1)] & i\exp[\tfrac{1}{2}i(2\theta_2-\theta-\theta_1)] \\ -i\exp[-\tfrac{1}{2}i(2\theta_2-\theta-\theta_1)] & -\exp[\tfrac{1}{2}i(\theta-\theta_1)] \end{bmatrix}.$$

Thus for $n=2$, a path-summation transition amplitude can be made identical to that of quantum mechanics, *even if the limit $\epsilon\to 0$ is not taken.* This suggests the possibility of formulating quantum mechanics in terms of path summations involving a fundamental time unit ϵ which is not set equal to zero; however, we will not pursue this any further here.

When n is even and the constraint equations (3.3) cannot be satisfied, one can still express the transition amplitude in path-summation form by converting the problem to $n+1$ dimensions. The new Hamiltonian's first n rows and columns are taken to be identical to those of the n-dimensional Hamiltonian. The $(n+1)$st row and the $(n+1)$st column are taken to be zero. Since the new Hamiltonian has an odd number of dimensions, the mathematical difficulty we have encountered is overcome. Moreover, the physical problem is unchanged, since no quantum transitions are possible from a state in the original n-dimensional space to the $(n+1)$st state, or vice versa [however, the $(n+1)$st state *does* participate in the path summation].

Thus we can produce a path-summation expression for the transition amplitude for any finite-dimensional quantum system.

IV. CONCLUDING REMARKS

An extension of the results of Sec. III to quantum systems with a countably infinite or uncountably infinite number of basis states can encounter difficulties. We have no proof of the existence of the formal extensions of expressions (2.7) and (2.13) to such systems. Moreover, even if they should exist, a real exponent in a path-summation expression does not guarantee that it bears a simple relationship to the classical action. Nonetheless, we believe that this approach can be fruitful. For example, we have been able to use these results to show[3] (at least formally) that a path-summation expression in which an arbitrary classical Hamiltonian is expressed in terms of classical harmonic-oscillator action-angle variables yields the transition amplitude for a related quantized Hamiltonian operator between harmonic-oscillator energy eigenstates. However, here we will content ourselves with showing how the usual phase-space path-summation expression described in the Introduction can be recovered by applying the procedures of Sec. II.

We set $x \equiv r\lambda$ (λ is an infinitesmal length), p

$=\pm\hbar k/n\lambda$, and take the limit $\lambda\to 0$, $n\to\infty$, $n\lambda\to L$ (L is the length of the "box" in which vectors are normalized to one). In the limit $L\to\infty$, the path summation (2.7) becomes the path integral (1.15), with S_1, S_2 given by (2.9):

$$S_2(x,p;\tfrac{1}{2}\epsilon)=-S_1(p,x;-\tfrac{1}{2}\epsilon)$$
$$=xp-\tfrac{1}{2}\epsilon\langle x|a|p\rangle+O(\epsilon^2)\,. \qquad (4.1)$$

In order that the Schrödinger equation be satisfied by the transition amplitude, $\langle x|a|p\rangle$ must satisfy (2.12):

$$\langle x|H|x_0\rangle=(4\pi\hbar)^{-1}\int_{-\infty}^{\infty}dp[\langle x|a|p\rangle+\langle x_0|a|p\rangle]\exp[ip(x-x_0)/\hbar]\,. \qquad (4.2)$$

We also require $\langle x|a|p\rangle$ to be real. The unique solution of these constraints, analogous to (2.13), is

$$\langle x|a|p\rangle=(\pi\hbar)^{-1}\int_{-\infty}^{\infty}dp_1\int_{-\infty}^{\infty}dx_1[1+\exp ip_1x_1/\hbar]^{-1}\operatorname{Tr}[\exp(-ip_1(X-x)/\hbar)H\exp(-ix_1(P-p)/\hbar)] \qquad (4.3)$$

Equation (4.3) can be evaluated for an arbitrary Hamiltonian. It is simplest to first cast the Hamiltonian in the symmetrical form (1.11). Insertion of (1.11) into (4.3), together with the continuum analog of (A.7) results in

$$\langle x|a|p\rangle=(2\pi\hbar)^{-1}\int_{-\infty}^{\infty}dp_1\int_{-\infty}^{\infty}dx_1\operatorname{Tr}\Big[\exp(-ip_1(X-x)/\hbar)\sum_i c_iG_i(X)F_i(P)\exp(-ix_1(P-p)/\hbar)\Big]. \qquad (4.4)$$

Straightforward evaluation of the trace yields the result

$$\langle x|a|p\rangle=(2\pi\hbar)^{-2}\int dp_1dx_1dp_2dx_2\exp(-ip_1(x_2-x)/\hbar)\sum_i c_iG_i(x_2)F_i(p_2)\exp(-ix_1(p_2-p)/\hbar)$$
$$=\sum_i c_iG_i(x)F_i(p)\,. \qquad (4.5)$$

Thus we obtain, as the continuum limit of our procedure for finite-dimensional systems, the results of Sec. II [compare (4.1) and (4.5) with (1.13)].

We have not given examples of how to handle infinite dimensional bases labeled by continuous indices of semi-infinite range, or a combination of discrete and continuous indices (such as the hydrogen-atom energy eigenstates). However, we believe that many of these cases can be treated by the methods shown here, as limiting cases of finite-dimensional quantum systems.

Incidentally, we remark that no one has shown how to express a transition amplitude between states belonging to *different* bases in path-summation form.

Finally, we would like to point out that, in view of the arbitrariness permitted to our Hamiltonians, it is possible to express unitary operators other than the time translation operator in path-summation form.

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APPENDIX

In this appendix we will find the real solution $\langle r|a|k\rangle$ that satisfies Eq. (2.12):

$$\langle r|H|s\rangle=(2n)^{-1}\sum_{k=0}^{n-1}[\langle r|a|k\rangle+\langle s|a|k\rangle]\times\exp[i2\pi k(r-s)/n]\,. \qquad (A1)$$

We first write (A1) as an operator equation. Noting that

$$n^{-1/2}\sum_{k=0}^{n-1}\langle r|a|k\rangle\exp[i2\pi k(r-s)/n]=\langle r|a\exp(i2\pi rK/n)|s\rangle\,, \qquad (A2)$$

and that if $\langle s|a|k\rangle$ is real,

$$\langle s|a|k\rangle=\langle k|a^\dagger|s\rangle\,, \qquad (A3)$$

then (A1) implies

$$H=2^{-1}n^{-1/2}\sum_{t=0}^{n-1}\{[|t\rangle\langle t|a\exp(i2\pi tK/n)]+[|t\rangle\langle t|a\exp(i2\pi tK/n)]^\dagger\}\,. \qquad (A4)$$

[We adopt the notation that letters preceding n in the alphabet (k,l,m) are labels for eigenvectors of K, while letters succeeding n in the alphabet ($r,s,t,$) are labels for eigenvectors of R.]

We now wish to evaluate

$$\operatorname{Tr}[\exp(-i2\pi kR/n)H\exp(-i2\pi rK/n)]\,. \qquad (A5)$$

This trace expression applied to the first term in (A4) yields

$$2^{-1}n^{-1/2}\sum_l\sum_t \exp(-i2\pi kt/n)\langle l|t\rangle\langle t|a|l\rangle \exp(i2\pi l(t-r)/n) = 2^{-1}\sum_l\sum_t\langle k|t\rangle\langle t|a|l\rangle\langle l|r\rangle = \tfrac{1}{2}\langle k|a|r\rangle\,. \tag{A6}$$

In order to evaluate the second term in (A4) it is useful to know the operator identity

$$\exp(-i2\pi rK/n)\exp(-i2\pi kR/n) = \exp(-i2\pi kR/n)\exp(-i2\pi rK/n)\exp(i2\pi rk/n)\,. \tag{A7}$$

With the help of (A7) and (A3), the trace applied to the second term in (A4) yields

$$2^{-1}n^{-1/2}\exp(i2\pi rk/n)\sum_l\sum_t \exp(-i2\pi l(t+r)/n)\langle l|a^\dagger|t\rangle\langle t|l\rangle\exp(-i2\pi kt/n) = 2^{-1}\exp(i2\pi rk/n)\sum_l\sum_t\langle k|t\rangle\langle l|a^\dagger|t\rangle\langle l|r\rangle = \tfrac{1}{2}\langle k|a|r\rangle\exp(i2\pi rk/n)\,. \tag{A8}$$

It follows from (A4), (A5), (A6), and (A8) that

$$\langle k|a|r\rangle = 2[1+\exp(i2\pi rk/n)]^{-1}\,\mathrm{Tr}[\exp(-i2\pi kR/n)H\exp(-i2\pi rK/n)]\,, \tag{A9}$$

provided the first factor on the right-hand side of (A9) is not infinite. If the factor is infinite and the trace does not vanish, no solution exists. If the factor is infinite, but the trace vanishes, we can take $\langle k|a|r\rangle = 0$.[19]

Thus the solution of (A1) is

$$\langle r|a|k\rangle = \frac{2}{n}\sum_{k_1=0}^{n-1}\sum_{r_1=0}^{n-1}[1+\exp(i2\pi r_1k_1/n)]^{-1}\,\mathrm{Tr}[\exp(-i2\pi k_1(R-r)/n)H\exp(-i2\pi r_1(K-k)/n)]\,. \tag{A10}$$

We must verify that this solution is real. If one takes the complex conjugate of (A10), replaces the summation indices k_1, r_1 by $k_1' \equiv n-k_1$, $r_1'\equiv n-r_1$, respectively, and utilizes (A7) to commute the exponential factors in the trace, one ends up once more with (A10).

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[2]Throughout this paper, for simplicity, we deal with only a single-position variable and a single-momentum variable. The results are easily extended to the case of any number of position and momentum variables. We also adopt the notation that X, P denote operators, and x, p denote classical variables (c numbers).

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