To reach a depth profounder still, and still
Profounder, in the fathomless abyss
WILLIAM COWPER (1731-1800), The Winter Morning Walk

12

New Path Integral Formula for Singular Potentials

In Chapter 8 we have seen that for systems with a centrifugal barrier, the Euclidean form of Feynman's original time-sliced path integral formula diverges for certain attractive barriers. This happens even if the quantum statistics of the systems is well defined. The same problem arises for a particle in an attractive Coulomb potential, and thus in any atomic system.

In this chapter we set up a new and more flexible path integral formula which is free of this problem for any singular potential. This has recently turned out to be the key for a simple solution of many other path integrals which were earlier considered intractable.

12.1 Path Collapse in Feynman's formula for the Coulomb System

The attractive Coulomb potential $V(r) = -e^2/r$ has a singularity at the coordinate origin $r = 0$. This singularity is weaker than that of the centrifugal barrier, but strong enough to cause a catastrophe in the Euclidean path integral. Recall that an attractive centrifugal barrier does not even possess a classical partition function. The same thing is true for the attractive Coulomb potential where formula (2.352) reads

$$Z_{\rm cl} = \int \frac{d^3x}{\sqrt{2\pi\hbar^2\beta/M}^3} \exp\left(\beta\frac{e^2}{r}\right).$$

The integral diverges near the origin. In addition, there is a divergence at large r. The leading part of the latter can be removed by subtracting the free-particle partition function and forming

$$Z'_{\rm cl} \equiv Z_{\rm cl} - Z_{\rm cl}\big|_{e=0} = \int \frac{d^3x}{\sqrt{2\pi\hbar^2\beta/M}^3} \left[\exp\left(\beta\frac{e^2}{r}\right) - 1\right], \tag{12.1}$$

leaving only a quadratic divergence. In a realistic many-body system with an equal number of oppositely charged particles, this disappears by screening effects. Thus we shall not worry about it any further and concentrate only on the remaining small-r divergence. In a real atom, this singularity is not present since the nucleus is not a point particle but occupies a finite volume. However, this "physical regularization" of the singularity is not required for quantum-mechanical stability. The Schrödinger equation is perfectly solvable for the singular pure $-e^2/r$ potential. We should therefore be able to recover the existing Schrödinger results from the path integral formalism without any short-distance regularization.

On the basis of Feynman's original time-sliced formula, this is impossible. If a path consists of a *finite* number of straight pieces, its Euclidean action

$$\mathcal{A} = \int_{\tau_a}^{\tau_b} d\tau \left[\frac{M}{2} \mathbf{x}'^2(\tau) - \frac{e^2}{r(\tau)} \right] \tag{12.2}$$

can be lowered indefinitely by a path with an almost stretched configuration which corresponds to a slowly moving particle sliding down into the $-e^2/r$ abyss. We call this phenomenon a *path collapse*. In nature, this catastrophe is prevented by quantum fluctuations. In order to understand how this happens, it is useful to reinterpret the paths in the Euclidean path integral as random lines parametrized by $\tau \in (\tau_a, \tau_b)$. Their distribution is governed by the "Boltzmann factor" $e^{-\mathcal{A}/\hbar}$, whose effective "quantum" temperature is $T_{\text{eff}} \equiv \hbar / k_B(\tau_b - \tau_a)$.[1] The logarithm of the Euclidean amplitude $(\mathbf{x}_b \tau_b | \mathbf{x}_a \tau_a)$ multiplied by $-T_{\text{eff}}$ defines a free energy

$$F = E - k_B T S$$

of the random line with fixed endpoints. The quantum fluctuations equip the path with a configurational entropy S. This must be sufficiently singular to produce a regular free energy bounded from below. Obviously, such a mechanism can only work if the exact path integral contains an *infinite* number of infinitesimally small sections. Only these can contain enough configurational entropy near the singularity to halt the collapse.

The variational approach in Section 5.10 has shown an important effect of the configurational entropy of quantum fluctuations. It smoothes the singular Coulomb potential producing an effective classical potential that is finite at the origin. A path collapse was avoided by defining the path integral as an infinite product of integrals over all Fourier coefficients. The infinitely high-frequency components were integrated out and this produced the desired stability. These high-frequency components are absent in a finitely time-sliced path with a finite number of pieces, where frequencies Ω_m are bounded by twice the inverse slice thickness $1/\epsilon$ [recall
ref(2.111) Eqs. (2.111), (2.112)].
lab(2.70) Unfortunately, the path measure used in the variational approach is unsuitable
est(2.80) ref(2.112) for exact calculations of nontrivial path integrals. Except for the free particle and

lab(2.71) est(2.81) [1]This amounts to viewing the path as a polymer with configurational fluctuations in space, a possibility which is a major topic in Chapters 15 and 16.

the harmonic oscillator, these are all based on solving a finite number of ordinary integrals in a time-sliced formula. We therefore need a more powerful time-sliced path integral formula which avoids a collapse in singular potentials.

For the Coulomb system, such a formula has been found in 1979 by Duru and Kleinert.[2] It has become the basis for solving the path integral of many other nontrivial systems. Here we describe the most general extension of this formula which will later be applied to a number of systems. For the attractive Coulomb potential and other singular potentials, such as attractive centrifugal barriers, it will not only halt the collapse, but also be the key to an analytic solution.

The derived stabilization is achieved by introducing a path-independent width of the time slices. If the path approaches an abyss, the widths decrease and the number of slices increases. This enables the configurational entropy of Eq. (12.3) to grow large enough to cancel the singularity in the energy. To see the cancellation mechanism, consider a random line with n links which has, on a simple cubic lattice in D dimensions, $(2D)^n$ configurations with an entropy

$$S = n\log(2D). \tag{12.3}$$

If the number of time slices n increases near the $-e^2/r$ singularity like const$/r$, then the entropy is proportional to $1/r$. A path section which slides down into the abyss must stretch itself to make the kinetic energy small. But then it gives up a certain entropy S, and this raises the free energy by $k_B T_{\rm eff} S$ according to (12.3). This compensates for the singularity in the potential and halts the collapse. The purpose of this chapter is to set up a path integral formula in which this stabilizing mechanism is at work.

It should be pointed out that no instability problem would certainly arise if we were to *define* the imaginary-time path integral for the time evolution amplitude in the continuum

$$(\mathbf{x}_b\tau_b|\mathbf{x}_a\tau_a) \equiv \int \mathcal{D}^D x(\tau) \int \frac{\mathcal{D}^D p(\tau)}{(2\pi\hbar)^D} \exp\left\{\frac{1}{\hbar}\int_{\tau_a}^{\tau_b} d\tau[i\mathbf{p}\dot{\mathbf{x}} - H(\mathbf{p},\mathbf{x})]\right\} \tag{12.4}$$

without any time slicing as the solution of the Schrödinger differential equation

$$(\hbar\partial_\tau + \hat{H})(\mathbf{x}\,\tau|\mathbf{x}_a\tau_a) = \hbar\delta(\tau-\tau_a)\delta^{(D)}(\mathbf{x}-\mathbf{x}_a) \tag{12.5}$$

[compare Eq. (1.308)]. After solving the Schrödinger equation $\hat{H}\psi_n(\mathbf{x}) = E_n\psi_n(\mathbf{x})$, the spectral representation (1.323) renders directly the amplitude (12.4).

All subtleties described above are due to the finite number of time slices in the path integral. As explained at the end of Section 2.1, the explicit sum over all paths is an essential ingredient of Feynman's global approach to the phenomena of

[2] I.H. Duru and H. Kleinert, Phys. Lett. B *84*, 30 (1979) (`http://www.physik.fu-berlin.de/~kleinert/65`); Fortschr. Phys. *30*, 401 (1982) (*ibid.*`http/83`). See also the historical remarks in the preface.

quantum fluctuations. Within this approach, the finite time slicing is essential for being able to perform this sum in any nontrivial system.

We now present a general solution to the stability problem of time-sliced quantum-statistical path integrals.

12.2 Stable Path Integral with Singular Potentials

Consider the fixed-energy amplitude (9.1) which is the local matrix element

$$(\mathbf{x}_b|\mathbf{x}_a)_E = \langle \mathbf{x}_b|\hat{R}|\mathbf{x}_a\rangle \tag{12.6}$$

of the resolvent operator (1.319):

ref(1.319)
lab(9.8)
est(9.15)

$$\hat{R} = \frac{i\hbar}{E - \hat{H} + i\eta}. \tag{12.7}$$

Recall that the $i\eta$-prescription ensures the causality of the Fourier transform of (12.6), making it vanish for $t_b < t_a$ [see the discussion after Eq. (1.327)].

The fixed-energy amplitude has poles of the form

$$(\mathbf{x}_b|\mathbf{x}_a)_E = \sum_n \frac{i\hbar}{E - E_n + i\eta}\psi_n(\mathbf{x}_b)\psi_n^*(\mathbf{x}_a) + \dots$$

at the bound-state energies, and a cut along the continuum part of the energy spectrum. The energy integral over the discontinuity across the singularities yields the completeness relation (1.330).

The new path integral formula is based on the following observation. If the system possesses a Feynman path integral for the time evolution amplitude, it does so also for the fixed-energy amplitude. This is seen after rewriting the latter as an integral

$$(\mathbf{x}_b|\mathbf{x}_a)_E = \int_{t_a}^{\infty} dt_b \langle \mathbf{x}_b|\hat{U}_E(t_b - t_a)|\mathbf{x}_a\rangle \tag{12.8}$$

involving the modified time evolution operator

$$\hat{U}_E(t) \equiv e^{-it(\hat{H}-E)/\hbar}, \tag{12.9}$$

that is associated with the modified Hamiltonian

$$\hat{H}_E \equiv \hat{H} - E. \tag{12.10}$$

Obviously, as long as the matrix elements of the ordinary time evolution operator $\hat{U}(t) = e^{-it\hat{H}/\hbar}$ can be represented by a time-sliced Feynman path integral, the same is true for the matrix elements of the modified operator $\hat{U}_E(t) = e^{-it\hat{H}_E/\hbar}$. Its explicit form is obtained, as in Section 2.1, by slicing the t-variable into $N+1$ pieces, factorizing $\exp(-it\hat{H}_E/\hbar)$ into the product of $N+1$ factors,

$$e^{-it\hat{H}_E/\hbar} = e^{-i\epsilon\hat{H}_E/\hbar} \cdots e^{-i\epsilon\hat{H}_E/\hbar}, \tag{12.11}$$

and inserting a sequence of N completeness relations

$$\prod_{n=1}^{N} \int d^D x_n |\mathbf{x}_n\rangle\langle\mathbf{x}_n| = 1 \tag{12.12}$$

(omitting the continuum part of the spectrum). In this way, we have arrived at the path integral for the time-sliced amplitude with $t_b - t_a = \epsilon(N+1)$

$$\langle\mathbf{x}_b|\hat{U}_E^N(t_b - t_a)|\mathbf{x}_a\rangle = \prod_{n=1}^{N}\left[\int d^D x_n\right]\prod_{n=1}^{N+1}\left[\int\frac{d^D p_n}{(2\pi\hbar)^D}\right]\exp\left(\frac{i}{\hbar}A_E^N\right), \tag{12.13}$$

where A_E^N is the sliced action

$$A_E^N = \sum_{n=1}^{N+1}\left\{\mathbf{p}_n(\mathbf{x}_n - \mathbf{x}_{n-1}) - \epsilon[H(\mathbf{p}_n,\mathbf{x}_n) - E]\right\}. \tag{12.14}$$

In the limit of large N at fixed $t_b - t_a = \epsilon(N+1)$, this defines the path integral

$$\langle\mathbf{x}_b|\hat{U}_E(t)|\mathbf{x}_a\rangle = \int\mathcal{D}^D x(t')\int\frac{\mathcal{D}^D p(t')}{(2\pi\hbar)^D}\exp\left\{\frac{i}{\hbar}\int_0^t dt'[\mathbf{p}\dot{\mathbf{x}}(t') - H_E(\mathbf{p}(t'),\mathbf{x}(t'))]\right\}. \tag{12.15}$$

It is easy to derive a finite-N approximation also for the fixed-energy amplitude $(\mathbf{x}_b|\mathbf{x}_a)_E$ of Eq. (12.8). The additional integral over $t_b > t_a$ can be approximated at the level of a finite N by an integral over the slice thickness ϵ:

$$\int_{t_a}^{\infty} dt_b = (N+1)\int_0^{\infty} d\epsilon. \tag{12.16}$$

The resulting finite-N approximation to the fixed-energy amplitude,

$$(\mathbf{x}_b|\mathbf{x}_a)_E^N \equiv (N+1)\int_0^{\infty} d\epsilon\langle\mathbf{x}_b|\hat{U}_E^N(\epsilon(N+1))|\mathbf{x}_a\rangle = \int_{t_a}^{\infty} dt_b\langle\mathbf{x}_b|\hat{U}_E^N(t_b - t_a)|\mathbf{x}_a\rangle, \tag{12.17}$$

converges against the correct limit $(\mathbf{x}_b|\mathbf{x}_a)_E$. As an example, take the free-particle case where

$$(\mathbf{x}_b|\mathbf{x}_a)_E^N = (N+1)\int_0^{\infty} d\epsilon\frac{1}{\sqrt{2\pi i(N+1)\epsilon\hbar/M}^D} \times\exp\left[i\frac{M}{2(N+1)\epsilon}(\mathbf{x}_b - \mathbf{x}_a)^2 + iE(N+1)\epsilon\right]. \tag{12.18}$$

After a trivial change of the integration variable, this is the same integral as in (1.343) whose result was given in (1.348) and (1.355), depending on the sign of the energy E. The N-dependence happens to disappear completely as observed in Section 2.2.5. In the general case of an arbitrary smooth potential, the convergence is still assured by the dominance of the kinetic term in the integral measure.

The time-sliced path integral formula for the fixed-energy amplitude $(\mathbf{x}_b|\mathbf{x}_a)_E$ given by (12.17), (12.13), (12.14) has apparently the same range of validity as the original Feynman path integral for the time evolution amplitude $(\mathbf{x}_b t_b|\mathbf{x}_a t_a)$. Thus, so far nothing has been gained. However, the new formula has an important advantage over Feynman's. Due to the additional time integration it possesses a new *functional* degree of freedom. This can be exploited to find a path-integral formula without collapse at imaginary times. The starting point is the observation that the resolvent operator $\hat{R}$ in Eq. (12.7) may be rewritten in the following three ways:

$$\hat{R} = \frac{i\hbar}{\hat{f}_l(E - \hat{H} + i\eta)}\hat{f}_l, \tag{12.19}$$

or

$$\hat{R} = \hat{f}_r\frac{i\hbar}{(E - \hat{H} + i\eta)\hat{f}_r}, \tag{12.20}$$

or, more generally,

$$\hat{R} = \hat{f}_r\frac{i\hbar}{\hat{f}_l(E - \hat{H} + i\eta)\hat{f}_r}\hat{f}_l, \tag{12.21}$$

where $\hat{f}_l, \hat{f}_r$ are arbitrary operators which may depend on $\hat{\mathbf{p}}$ and $\hat{\mathbf{x}}$. They are called *regulating functions*. In the subsequent discussion, we shall avoid operator-ordering subtleties by assuming $\hat{f}_l, \hat{f}_r$ to depend only on $\hat{\mathbf{x}}$, although the general case can also be treated along similar lines. Moreover, in the specific application to follow in Chapters 13 and 14, the operators $\hat{f}_l, \hat{f}_r$ to be assumed consist of two different powers of one and the same operator $\hat{f}$, i.e.,

$$\hat{f}_l = \hat{f}^{1-\lambda}, \quad \hat{f}_r = \hat{f}^{\lambda}, \tag{12.22}$$

whose product is

$$\hat{f}_l\hat{f}_r = \hat{f}. \tag{12.23}$$

Taking the local matrix elements of (12.21) renders the alternative representations for the fixed-energy amplitude

$$\langle\mathbf{x}_b|\hat{R}|\mathbf{x}_a\rangle = (\mathbf{x}_b|\mathbf{x}_a)_E = \int_{s_a}^{\infty} ds_b\langle\mathbf{x}_b|\hat{\mathcal{U}}_E(s_b - s_a)|\mathbf{x}_a\rangle, \tag{12.24}$$

where $\hat{\mathcal{U}}_E(s)$ is the generalization of the modified time evolution operator (12.9), to be called the *pseudotime evolution operator*,

$$\hat{\mathcal{U}}_E(s) \equiv f_r(\mathbf{x})e^{-isf_l(\mathbf{x})(\hat{H}-E)f_r(\mathbf{x})}f_l(\mathbf{x}). \tag{12.25}$$

The operator in the exponent,

$$\hat{\mathcal{H}}_E \equiv f_l(\mathbf{x})(\hat{H} - E)f_r(\mathbf{x}), \tag{12.26}$$

may be considered as an auxiliary Hamiltonian which drives the state vectors $|\mathbf{x}\rangle$ of the system along a pseudotime s-axis, with the operator $e^{-is\hat{\mathcal{H}}_E(\mathbf{p},\mathbf{x})/\hbar}$. Note that $\hat{\mathcal{H}}_E$ is in general not Hermitian, in which case $\hat{\mathcal{U}}_E(s)$ is not unitary.

As usual, we convert the expression (12.24) into a path integral by slicing the pseudotime interval $(0, s)$ into $N+1$ pieces, factorizing $\exp(-is\hat{\mathcal{H}}_E/\hbar)$ into a product of $N + 1$ factors, and inserting a sequence of N completeness relations. The result is the approximate integral representation for the fixed-energy amplitude,

$$(\mathbf{x}_b|\mathbf{x}_a)_E \;\;\approx\;\; (N+1)\int_0^\infty d\epsilon_s \langle \mathbf{x}_b|\hat{\mathcal{U}}_E^N\left(\epsilon_s(N+1)\right)|\mathbf{x}_a\rangle, \tag{12.27}$$

with the path integral for the pseudotime-sliced amplitude

$$\langle \mathbf{x}_b|\hat{\mathcal{U}}_E^N\left(\epsilon_s(N+1)\right)|\mathbf{x}_a\rangle = f_r(\mathbf{x}_b)f_l(\mathbf{x}_a)\prod_{n=1}^{N}\left[\int d^Dx_n\right]\prod_{n=1}^{N+1}\left[\int \frac{d^Dp_n}{(2\pi\hbar)^D}\right]e^{i\mathcal{A}_E^N/\hbar}, \tag{12.28}$$

whose time-sliced action reads

$$\mathcal{A}_E^N = \sum_{n=1}^{N+1}\left\{\mathbf{p}_n(\mathbf{x}_n - \mathbf{x}_{n-1}) - \epsilon_s f_l(\mathbf{x}_n)[H(\mathbf{p}_n, \mathbf{x}_n) - E]f_r(\mathbf{x}_n)\right\}. \tag{12.29}$$

These equations constitute the desired generalization of the formulas (12.13)–(12.17). In the limit of large N, we can write the fixed-energy amplitude as an integral

$$(\mathbf{x}_b|\mathbf{x}_a)_E = \int_0^\infty dS \langle \mathbf{x}_b|\hat{\mathcal{U}}_E(S)|\mathbf{x}_a\rangle \tag{12.30}$$

over the amplitude

$$\langle \mathbf{x}_b|\hat{\mathcal{U}}_E(S)|\mathbf{x}_a\rangle = f_r(\mathbf{x}_b)f_l(\mathbf{x}_a)\int\mathcal{D}x(s)\int\frac{\mathcal{D}p(s)}{2\pi\hbar}\exp\left\{\frac{i}{\hbar}\int_0^S ds[\mathbf{p}\mathbf{x}' - \mathcal{H}_E(\mathbf{p}, \mathbf{x})]\right\}. \tag{12.31}$$

The prime on $\mathbf{x}(s)$ denotes the derivative with respect to the pseudotime s.

For a standard Hamiltonian of the form

$$H = T(\mathbf{p}) + V(\mathbf{x}), \tag{12.32}$$

with the kinetic energy

$$T(\mathbf{p}) = \frac{\mathbf{p}^2}{2M}, \tag{12.33}$$

the momenta $\mathbf{p}_n$ in (12.28) can be integrated out and we obtain the configuration space path integral

$$\langle \mathbf{x}_b|\hat{\mathcal{U}}_E^N\left(\epsilon_s(N+1)\right)|\mathbf{x}_a\rangle = \frac{f_r(\mathbf{x}_b)f_l(\mathbf{x}_a)}{\sqrt{2\pi i\epsilon_s f_l(\mathbf{x}_b)f_r(\mathbf{x}_a)\hbar/M}^D} \times \prod_{n=1}^{N}\left[\int \frac{d^D x_n}{\sqrt{2\pi i\epsilon_s f(\mathbf{x}_n)\hbar/M}^D}\right] e^{i\mathcal{A}_E^N/\hbar}, \tag{12.34}$$

with the sliced action

$$\mathcal{A}_E^N = \sum_{n=1}^{N+1}\left\{\frac{M}{2\epsilon_s f_l(\mathbf{x}_n)f_r(\mathbf{x}_{n-1})}(\mathbf{x}_n-\mathbf{x}_{n-1})^2 - \epsilon_s f_l(\mathbf{x}_n)[V(\mathbf{x}_n)-E]f_r(\mathbf{x}_{n-1})\right\}. \tag{12.35}$$

In the limit of large N, this may be written as a path integral

$$\langle \mathbf{x}_b|\hat{\mathcal{U}}_E(S)|\mathbf{x}_a\rangle = f_r(\mathbf{x}_b)f_l(\mathbf{x}_a)\int\mathcal{D}x(s)\exp\left\{\frac{i}{\hbar}\int_0^S ds\left[\frac{M}{2f_lf_r}\mathbf{x}'^2 - f_l(V-E)f_r\right]\right\}, \tag{12.36}$$

with the slicing specification (12.35).

The path integral formula for the fixed-energy amplitude based on Eqs. (12.30) and (12.36) is independent of the particular choice of the functions $f_l(\mathbf{x}), f_r(\mathbf{x})$, just like the most general operator expression for the resolvent (12.21). Feynman's original time-sliced formula is, of course, recovered with the special choice $f_l(\mathbf{x}) \equiv f_r(\mathbf{x}) \equiv 1$.

When comparing (12.25) with (12.9), we see that for each infinitesimal pseudotime slice, the thickness of the true time slices has the space-dependent value

$$dt = ds f_l(\mathbf{x}_n)f_r(\mathbf{x}_{n-1}). \tag{12.37}$$

The freedom in choosing $f(\mathbf{x})$ amounts to an *invariance under path-dependent time reparametrizations* of the fixed-energy amplitude (12.30). Note that the invariance is exact in the general operator formula (12.21) for the resolvent and in the continuum path integral formula based on (12.30) and (12.36). However, the finite pseudotime slicing in (12.34), (12.35) used to define the path integral, destroys this invariance. At a finite value of N, different choices of $f(\mathbf{x})$ produce different approximations to the matrix element of the operator $\hat{\mathcal{U}}_E(s) = f_r(\hat{\mathbf{x}})e^{-is\hat{\mathcal{H}}_E(\hat{\mathbf{p}},\hat{\mathbf{x}})/\hbar}f_l(\hat{\mathbf{x}})$. Their quality can vary greatly. In fact, if the potential is singular and the regulating functions $f_r(\mathbf{x}), f_l(\mathbf{x})$ are not suitably chosen, the Euclidean pseudotime-sliced expression may not exist at all. This is what happens in the Coulomb system if the functions $f_l(\mathbf{x})$ and $f_r(\mathbf{x})$ are both chosen to be unity as in Feynman's path integral formula.

The new reparametrization freedom gained by the functions $f_l(\mathbf{x}), f_r(\mathbf{x})$ is therefore not just a luxury. It is *essential* for stabilizing the Euclidean time-sliced orbital fluctuations in singular potentials.

In the case of the Coulomb system, any choice of the regulating functions $f_l(\mathbf{x}), f_r(\mathbf{x})$ with $f(\mathbf{x}) = r$ leads to a regular auxiliary Hamiltonian $\mathcal{H}_E$, and the path integral expressions (12.27)–(12.36) are all well defined. This was the important discovery of Duru and Kleinert in 1979, to be described in detail in Chapter 13, which has made a large class of previously non-existing Feynman path integrals solvable. By a similar Duru-Kleinert transformation with $f_l(\mathbf{x}), f_r(\mathbf{x})$ with $f(\mathbf{x}) = \sqrt{f_l(\mathbf{x})f_r(\mathbf{x})} = r^2$, the earlier difficulties with the centrifugal barrier are resolved, as will be seen in Chapter 14.

12.3 Time-Dependent Regularization

Before treating specific cases, let us note that there exists a further generalization of the above path integral formula which is useful in systems with a time-dependent Hamiltonian $H(\mathbf{p}, \mathbf{x}, t)$. There we introduce an auxiliary Hamiltonian

$$\hat{\mathcal{H}} = f_l(\mathbf{x}, t)[H(\hat{\mathbf{p}}, \mathbf{x}, t) - \hat{E}]f_r(\mathbf{x}, t), \tag{12.38}$$

where $\hat{E}$ is the differential operator for the energy which is canonically conjugate to the time t:

$$\hat{E} \equiv i\hbar\partial_t. \tag{12.39}$$

The auxiliary Hamiltonian acts on an extended Hilbert space, in which the states are localized in space *and* time. These states will be denoted by $|\mathbf{x}, t\}$. They satisfy the orthogonality and completeness relations

$$\{\mathbf{x}\,t|\mathbf{x}'\,t'\} = \delta^{(D)}(\mathbf{x} - \mathbf{x}')\delta(t - t'), \tag{12.40}$$

and

$$\int d^D x \int dt |\mathbf{x}\,t\}\{\mathbf{x}\,t| = 1, \tag{12.41}$$

respectively. By construction, the Hamiltonian $\mathcal{H}$ does not depend explicitly on the pseudotime s. The pseudotime evolution operator is therefore obtained by a simple exponentiation, as in (12.25),

$$\hat{\mathcal{U}}(s) \equiv f_r(\mathbf{x}, t)e^{-isf_l(\mathbf{x},t)(\hat{H}-\hat{E})f_r(\mathbf{x},t)}f_l(\mathbf{x}, t). \tag{12.42}$$

The derivation of the path integral is then completely analogous to the time-independent case. The operator (12.42) is sliced into $N + 1$ pieces, and N completeness relations (12.41) are inserted to obtain the path integral

$$\begin{aligned}\{\mathbf{x}_b t_b|\hat{\mathcal{U}}^N(s)|\mathbf{x}_a t_a\} &= f_r(\mathbf{x}_b, t_b)f_l(\mathbf{x}_a, t_a)\\ &\quad\times \prod_{n=1}^{N}\left[\int d^D x_n dt_n\right]\prod_{n=1}^{N+1}\left[\int \frac{d^D p_n}{(2\pi\hbar)^D}\frac{dE_n}{2\pi\hbar}\right]e^{i\mathcal{A}^N/\hbar},\end{aligned} \tag{12.43}$$

with the pseudotime-sliced action

$$\begin{aligned}\mathcal{A}^N &= \sum_{n=1}^{N+1}\{\mathbf{p}_n(\mathbf{x}_n - \mathbf{x}_{n-1}) - E_n(t_n - t_{n-1})\\ &\qquad - f_l(\mathbf{x}_n, t_n)\left[H(\mathbf{p}_n, \mathbf{x}_n, t_n) - E_n\right]f_r(\mathbf{x}_{n-1}, t_{n-1})\},\end{aligned} \tag{12.44}$$

where $\mathbf{x}_b = \mathbf{x}_{N+1}$, $t_b = t_{N+1}$; $\mathbf{x}_a = \mathbf{x}_0$, $t_a = t_0$. This describes orbital fluctuations in the phase space of spacetime which contains fluctuating worldlines $\mathbf{x}(s), t(s)$ and their canonically conjugate spacetime $\mathbf{p}(s), E(s)$. In the limit $N \to \infty$ we write this as

$$\begin{aligned}\{\mathbf{x}_b t_b|\hat{\mathcal{U}}(S)|\mathbf{x}_a t_a\} &= f_r(\mathbf{p}_b, \mathbf{x}_b, t_b) f_l(\mathbf{p}_a, \mathbf{x}_a, t_a) \\ &\times \int \mathcal{D}^D x(s)\mathcal{D}t(s) \int \frac{\mathcal{D}^D p(s)}{(2\pi\hbar)^D} \frac{\mathcal{D}E(s)}{2\pi\hbar} e^{i\mathcal{A}/\hbar},\end{aligned} \tag{12.45}$$

with the continuous action

$$\begin{aligned}\mathcal{A}[\mathbf{p}, \mathbf{x}, E, t] &= \int_0^S ds \{\mathbf{p}(s)\mathbf{x}'(s) - E(s)t'(s) \\ &-f_l(\mathbf{p}(s), \mathbf{x}(s), t(s)) \left[H(\mathbf{p}(s), \mathbf{x}(s), t(s)) - E(s)\right] f_r(\mathbf{p}(s), \mathbf{x}(s), t(s))\}.\end{aligned} \tag{12.46}$$

In the pseudotime-sliced formula (12.43), we can integrate out all intermediate energy variables E_n and obtain

$$\begin{aligned}\{\mathbf{x}_b t_b|\hat{\mathcal{U}}(S)|\mathbf{x}_a t_a\} = \prod_{n=1}^{N} \left[\int d^D x_n\right] \prod_{n=1}^{N+1} \left[\int \frac{d^D p_n}{(2\pi\hbar)^D}\right] \\ \times \delta\left(t_b - t_a - \epsilon_s \sum_{n=1}^{N+1} f_l(\mathbf{p}_n, \mathbf{x}_n, t_n) f_r(\mathbf{p}_{n-1}, \mathbf{x}_{n-1}, t_{n-1})\right) e^{i\tilde{\mathcal{A}}^N/\hbar}\end{aligned} \tag{12.47}$$

with the action

$$\tilde{\mathcal{A}}^N = \sum_{n=1}^{N+1} [\mathbf{p}_n(\mathbf{x}_n - \mathbf{x}_{n-1}) - \epsilon_s f_l(\mathbf{p}_n \mathbf{x}_n, t_n) H(\mathbf{p}_n, \mathbf{x}_n, t_n) f_r(\mathbf{p}_{n-1}, \mathbf{x}_{n-1}, t_{n-1})]. \tag{12.48}$$

This looks just like an ordinary time-sliced action with a time-dependent Hamiltonian. The constant width of the time slices $\epsilon = (t_b - t_a)/(N + 1)$, however, has now become variable and depends on phase space and time:

$$\epsilon \to \epsilon_s f_l(\mathbf{p}_n \mathbf{x}_n, t_n) f_r(\mathbf{p}_{n-1}, \mathbf{x}_{n-1}, t_{n-1}). \tag{12.49}$$

The δ-function in (12.47) ensures the correct relation between the pseudotime s and the physical time t. In the continuum limit we may write (12.47) as

$$\{\mathbf{x}_b t_b|\hat{\mathcal{U}}(S)|\mathbf{x}_a t_a\} = \int \mathcal{D}^D x(s) \int \frac{\mathcal{D}^D p(s)}{(2\pi\hbar)^D} \delta(t_b - t_a - \int_0^S ds\, f(\mathbf{x}, t)) e^{i\tilde{\mathcal{A}}/\hbar}, \tag{12.50}$$

with the pseudotime action

$$\tilde{\mathcal{A}}[\mathbf{p}, \mathbf{x}, t] = \int_0^S ds \left[\mathbf{p}\mathbf{x}' - f_l(\mathbf{x}, t) H(\mathbf{p}, \mathbf{x}, t) f_r(\mathbf{x}, t)\right], \tag{12.51}$$

which is a functional of the s-dependent paths $\mathbf{x}(s), \mathbf{p}(s), t(s)$. Note that in the continuum formula, the splitting of the regulating function $f(\mathbf{x}, t)$ into $f_l(\mathbf{x}, t)$ and

$f_r(\mathbf{x},t)$ according to the parameter λ in Eq. (12.22) cannot be expressed properly since f_l, H, and f_r are commuting c-number functions. We have written them in a way indicating their order in the time-sliced expressions (12.47), (12.48).

The integral over S yields the original time evolution amplitude

$$(\mathbf{x}_b t_a|\mathbf{x}_a t_a) = \int_0^\infty dS\{\mathbf{x}_b t_b|\hat{\mathcal{U}}(S)|\mathbf{x}_a t_a\} = \left\{\mathbf{x}_b t_b\left|\frac{i\hbar}{\hat{H}-\hat{E}}\right|\mathbf{x}_a t_a\right\}. \tag{12.52}$$

Indeed, by Fourier decomposing the scalar products $\{\mathbf{x}_b t_b|\mathbf{x}_a t_a\}$,

$$\{\mathbf{x}_b t_b|\mathbf{x}_a t_a\} = \int \frac{d^D p}{(2\pi\hbar)^D}\int\frac{dE}{2\pi\hbar}e^{i\mathbf{p}(\mathbf{x}_b-\mathbf{x}_a)/\hbar - iE(t_b-t_a)/\hbar}, \tag{12.53}$$

we see that the right-hand side satisfies the same Schrödinger equation as the left-hand side:

$$[H(-i\hbar\partial_{\mathbf{x}},\mathbf{x},t)-i\hbar\partial_t]\,(\mathbf{x}\,t|\mathbf{x}_a t_a) = -i\hbar\delta^{(D)}(\mathbf{x}-\mathbf{x}_a)\delta(t-t_a) \tag{12.54}$$

[recall (1.308) and (12.5)]. If the δ-function in (12.47) is written as a Fourier integral, ref(1.308)
we obtain a kind of spectral decomposition of the amplitude (12.52), lab(x1.327)
est(1.327)

$$(\mathbf{x}_b t_a|\mathbf{x}_a t_a) \;=\; \int_{-\infty}^{\infty} dE e^{-iE(t_b-t_a)/\hbar}\int_0^\infty dS\{\mathbf{x}_b t_b|\hat{\mathcal{U}}_E(S)|\mathbf{x}_a t_a\}, \tag{12.55}$$

with the pseudotime evolution amplitude:

$$\hat{\mathcal{U}}_E(s) \equiv f_r(\hat{\mathbf{p}},\mathbf{x},t)e^{-isf_l(\hat{\mathbf{p}},\mathbf{x},t)(\hat{H}-E)f_r(\hat{\mathbf{p}},\mathbf{x},t)}f_l(\hat{\mathbf{p}},\mathbf{x},t). \tag{12.56}$$

12.4 Relation to Schrödinger Theory. Wave Functions

For completeness, consider also the ordinary Schrödinger quantum mechanics described by the pseudo-Hamiltonian $\hat{\mathcal{H}}$. This operator is the generator of translations of the system along the pseudotime axis s. Let $\phi(\mathbf{x},t,s)$ be a solution of the pseudotime Schrödinger equation

$$\mathcal{H}(\hat{\mathbf{p}},\mathbf{x},\hat{E},t)\phi(\mathbf{x},t,s) = i\hbar\partial_s\phi(\mathbf{x},t,s), \tag{12.57}$$

written more explicitly as

$$f_l(\mathbf{x},t)\,[H(\hat{\mathbf{p}},\mathbf{x},t)-i\hbar\partial_t]\,f_r(\mathbf{x},t)\phi(\mathbf{x},t,s) = i\hbar\partial_s\phi(\mathbf{x},t,s). \tag{12.58}$$

Since the left-hand side is independent of s, the s-dependence of $\phi(\mathbf{x},t,s)$ can be factored out:

$$\phi(\mathbf{x},t,s) = \phi_{\mathcal{E}}(\mathbf{x},t)e^{-i\mathcal{E}s/\hbar}. \tag{12.59}$$

If H is independent of the time t, it is always possible to stabilize the path integral by a time-independent reparametrization function $f(\mathbf{x})$. Then we remove an oscillating factor $e^{-iEt/\hbar}$ from $\phi_{\mathcal{E}}(\mathbf{x},t)$ and factorize

$$\phi_{\mathcal{E}}(\mathbf{x},t) = \phi_{\mathcal{E},E}(\mathbf{x})e^{-iEt/\hbar}. \tag{12.60}$$

This leaves us with the time- and pseudotime-independent equation

$$\begin{aligned}\mathcal{H}(\hat{\mathbf{p}},\mathbf{x},E)\phi_{\mathcal{E},E}(\mathbf{x}) &= f_l(\mathbf{x})\left[H(\hat{\mathbf{p}},\mathbf{x})-E\right]f_r(\mathbf{x})\phi_{\mathcal{E},E}(\mathbf{x}) \\ &= \mathcal{E}\phi_{\mathcal{E},E}(\mathbf{x}).\end{aligned} \tag{12.61}$$

For each value of E, there will be a different spectrum of eigenvalues $\mathcal{E}_n$. This is indicated by writing the eigenvalues $\mathcal{E}_n$ as $\mathcal{E}_n(E)$ and the associated eigenstates $\phi_{\mathcal{E}_n,E(\mathbf{x})}$ as $\phi_{\mathcal{E}_n(E)}$.

Suppose that we possess a complete set of such eigenstates at a fixed energy E labeled by a quantum number n (which is here assumed to take discrete values although it may include continuous values, as usual). We can then write down a spectral representation for the local matrix elements of the pseudotime evolution amplitude (12.25):

$$\langle\mathbf{x}_b|\hat{\mathcal{U}}_E(S)|\mathbf{x}_a\rangle = f_r(\mathbf{x}_b)f_l(\mathbf{x}_a)\sum_n \phi_{\mathcal{E}_n(E)}(\mathbf{x}_b)\phi^*_{\mathcal{E}_n(E)}(\mathbf{x}_a)e^{-iS\mathcal{E}_n(E)/\hbar}. \tag{12.62}$$

From this we find the expansion for the fixed-energy amplitude (12.24):

$$(\mathbf{x}_b|\mathbf{x}_a)_E = f_r(\mathbf{x}_b)f_l(\mathbf{x}_a)\sum_n \phi_{\mathcal{E}_n(E)}(\mathbf{x}_b)\phi^*_{\mathcal{E}_n(E)}(\mathbf{x}_a)\frac{i\hbar}{\mathcal{E}_n(E)}.$$

The time evolution amplitude is given by the Fourier transform

$$(\mathbf{x}_bt_b|\mathbf{x}_at_a) = f_r(\mathbf{x}_b)f_l(\mathbf{x}_a)\int_{-\infty}^{\infty}\frac{dE}{2\pi\hbar}e^{iE(t_b-t_a)/\hbar}\sum_n \phi_{\mathcal{E}_n(E)}(\mathbf{x}_b)\phi^*_{\mathcal{E}_n(E)}(\mathbf{x}_a)\frac{i\hbar}{\mathcal{E}_n(E)}. \tag{12.63}$$

This is to be compared with the usual spectral representation of this amplitude for the time-independent Hamiltonian $\hat{H}$

$$(\mathbf{x}_bt_b|\mathbf{x}_at_a) = \sum_n \psi_n(\mathbf{x}_b)\psi_n^*(\mathbf{x}_a)e^{-iE_n(t_b-t_a)/\hbar}, \tag{12.64}$$

where $\psi_n(\mathbf{x})$ are the solutions of the ordinary time-independent Schrödinger equation:

$$H(\hat{\mathbf{p}},\mathbf{x})\psi_n(\mathbf{x}) = E_n\psi_n(\mathbf{x}). \tag{12.65}$$

The relation between the two representations (12.63) and (12.64) is found by observing that for the energy E coinciding with the energy E_n, the eigenvalue $\mathcal{E}_n(E)$ vanishes, i.e., $i\hbar/\mathcal{E}_n(E)$ has poles at $E=E_n$ of the form

$$\frac{i\hbar}{\mathcal{E}_n(E)} \approx \frac{1}{\mathcal{E}'_n(E_n)}\frac{i\hbar}{E-E_n+i\eta}. \tag{12.66}$$

These contribute to the energy integral in (12.63) with a sum

$$(\mathbf{x}_bt_b|\mathbf{x}_at_a) \sim f_r(\mathbf{x}_b)f_l(\mathbf{x}_a)\sum_n \phi_{\mathcal{E}_n(E_n)}(\mathbf{x}_b)\phi^*_{\mathcal{E}_n(E_n)}(\mathbf{x}_a)e^{-iE_n(t_b-t_a)/\hbar}. \tag{12.67}$$

A comparison with (12.64) shows the relation between the bound-state wave functions of the ordinary and the pseudotime Schrödinger equation. In general, the function $i\hbar/\mathcal{E}_n(E)$ also has cuts whose discontinuities contain the continuum wave functions of the Schrödinger equation (12.65).

These observations will become more transparent in Section 13.8 when treating in detail the bound and continuum wave functions of the Coulomb system.

Notes and References

The general path integral formula with time reparametrization was introduced by
H. Kleinert, Phys. Lett. A **120**, 361 (1987) (`http://www.physik.fu-berlin.de/~kleinert/163`).
The stability aspects are discussed in
H. Kleinert, Phys. Lett. B **224**, 313 (1989) (*ibid.*`http/195`).