

# Hamiltonian path integrals

L. V. Prokhorov

Leningrad State University

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The properties of path integrals associated with the allowance for nonstandard terms reflecting the operator nature of the canonical variables are considered. Rules for treating such terms ("equivalence rules") are formulated. Problems with a boundary, the behavior of path integrals under canonical transformations, and the problem of quantization of dynamical systems with constraints are considered in the framework of the method.

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## INTRODUCTION

Path integrals, which were invented by Feynman in the forties<sup>1,2</sup> (Dirac<sup>3</sup> came very close to their formulation), have become an important tool of modern theoretical physics. They find application not only where it is necessary to give a quantum description of systems with an infinite (or very large) number of degrees of freedom, for example, in quantum field theory or solid-state theory, but also in problems of ordinary quantum mechanics. Moreover, there is a tendency to reformulate ordinary quantum-mechanical problems (for example, a particle in a box<sup>4</sup>) in the language of path integrals.

The popularity of path integrals in quantum field theory is due to the fact that they provide the mathematical formalism most adequate to the problem, making it possible to cast the expressions into a very compact form and, therefore, to avoid cumbersome calculations. But apart from these purely technical (though very important) advantages, the path-integral method opens up new possibilities for applications; for example, in the framework of the method one can construct naturally a quasiclassical approximation, which enables one to go beyond the limits of perturbation theory. In quantum mechanics, path integrals, being very perspicuous, enable one to reexamine old, well-known problems. Studies in this direction are helpful not only for revealing the possibilities of the method but also for better understanding of the formalism itself. The point is that despite the wide use of the "calculus of path integrals" (especially in the last decade), it has still not yet been adequately developed. Apart from the purely mathematical problems associated with the method, one must include here the problem of calculating the integrals. Essentially, and not counting the trivial cases, one only knows how to calculate Gaussian path integrals or path integrals that reduce to them.

Much less difficult, but very important for practical applications, are the questions concerning allowance within the formalism for the noncommutativity of operators, the behavior of path integrals under canonical transformations, and the formulation in this language of theories with constraints. They are important not only for quantum mechanics but also for quantum field theory. Some aspects of the last three questions are discussed in the present paper, which is devoted to

Hamiltonian path integrals in nonrelativistic quantum mechanics.

Besides the papers of Feynman,<sup>1</sup> we must recognize the key contributions made by Pauli,<sup>4</sup> Morette,<sup>5</sup> and DeWitt.<sup>6</sup> Starting from a remark of Feynman (Ref. 1, p. 185 of the Russian translation), and taking as his basis Van Vleck's paper<sup>7</sup> on the quasiclassical approximation for the wave function (see also Ref. 8),

$$\langle q(t) | q'(0) \rangle \approx c D^{1/2} \exp [iS(q, q')/\hbar]; D = \det \left| -\frac{\partial^2 S}{\partial q^i \partial q'^j} \right| \quad (1)$$

( $S$  is the classical action), Pauli proposed that (1) should be regarded as an exact expression for the propagator in the limit  $t \rightarrow 0$  ( $t$  is the time). This expression was introduced and justified independently in Ref. 5. In his lectures (1950–1951), Pauli also derived a Schrödinger equation satisfied by the function (1) in the limit  $t \rightarrow 0$  [(A.31) for  $g_{ij} = c_i \delta_{ij}$ ]. DeWitt generalized this result to the case of curvilinear coordinates. Two important points were brought out explicitly in DeWitt's paper of Ref. 6. First, the action  $S(q, q')$  was calculated up to terms  $(\Delta q)^4/t$  ( $t \rightarrow 0$ ,  $\Delta q = q - q'$ ),<sup>11</sup> and, second, it was pointed out that the method can be automatically extended to spaces with curvature (when the Hamiltonian is modified by addition of the term  $\hbar^2 R/12$ , where  $R$  is the scalar curvature).

The appearance in the action of the nonstandard terms of the type  $(\Delta q)^3/t$ ,  $(\Delta q)^4/t$ ,  $t \rightarrow 0$  ("extraterms") poses the question of how one should deal with them. McLaughlin and Schulman<sup>10</sup> showed that a theory with extraterms is equivalent to a theory without extraterms but with a modified potential, and they explicitly formulated the rules for constructing the new potential ("equivalence rules"). These rules were already contained explicitly in DeWitt's paper of Ref. 6.<sup>21</sup> The developed formalism enabled Gervais and Jevicki<sup>11</sup> to establish how a Lagrangian path integral, i.e., a path integral in configuration space, transforms under canonical point transformations (see also Ref. 12). In Refs. 13–15, the

<sup>11</sup>We should here mention the paper of Edwards and Gulyaev,<sup>9</sup> who studied the properties of a path integral in polar coordinates and, obviously unaware of Ref. 6, also concluded that it is necessary to take into account in the action higher powers of  $\Delta q$ .

<sup>21</sup>We mention that in one simple case the corresponding rule was formulated in Ref. 6 explicitly.

ideas of Pauli and DeWitt were used for quantization on a group space; their use in quantum field theory was discussed in Refs. 16 and 17. Cheng<sup>18</sup> made calculations parallel to those of Ref. 6 and obtained a Schrödinger equation using the equivalence rules; however, for some reason he ignored the factor  $D^{1/2}$  in (1).

The need to take into account not only the lowest powers of  $\Delta q$  is well known to mathematicians who study random (diffusion) processes. For example, if  $q(t)$  is the trajectory of a Brownian particle, the differential of the function  $f[q(t)]$  is

$$df(q) = f'(q) dq + \frac{1}{2} f''(q) dt \quad (2)$$

(Itô's formula), i.e.,

$$\int_{t'}^t f'(q) dq = f(q)|_{t'}^t - \frac{1}{2} \int_{t'}^t f''(q) dt. \quad (3)$$

Here, first,  $(dq)^2$  terms are taken into account and, second, the equivalence  $(dq)^2 \sim dt$  is in fact used. The appearance of expressions of the type (3) is, of course, due to the nondifferentiability of the trajectory of a Brownian particle (see Ref. 19).

The same circumstance is encountered in mathematical physics when equations are investigated by means of path integrals. In Ref. 20, Buslaev constructed an equation of Hamilton-Jacobi type (A.23) and solved it in the limit  $\varepsilon = t - t' \rightarrow 0$ , retaining the terms  $(\Delta q)^3/\varepsilon$  and  $(\Delta q)^4/\varepsilon$  (see also Ref. 21 in which the equivalence rules were essentially used).

Soon after the publication of Ref. 1, Feynman formulated quantum mechanics in the language of path integrals in phase space<sup>22</sup> ("Hamiltonian" path integrals). The same question was considered later in Refs. 23-25. Hamiltonian path integrals have attracted rather a lot of attention, for which there are several reasons. First, the standard method of quantization<sup>3</sup> is associated with Hamiltonian theory, and therefore the creation of such a formalism makes it possible to establish directly the connection between the standard and Feynman formulations of quantum mechanics. Further, in the Hamiltonian formalism the unitarity of the  $S$  matrix can be most readily verified. Finally, Hamiltonian path integrals are important for formulating gauge theories. In connection with the well-known gauge-fixing problems in the theory of Yang-Mills fields,<sup>26</sup> the desire to eliminate from the start all unphysical variables<sup>27, 28</sup> can be readily understood. This can be done in a natural manner in the Hamiltonian formalism, and therefore, if, as before, we wish to use all the advantages of the method of path integrals, a Hamiltonian formulation of the method is needed.

The Hamiltonian path integrals take their simplest form for systems with Lagrangians of the form  $\dot{q}^2/2 - V(q)$ . In this case, there is no operator-ordering problem, and the classical Hamiltonian occurs in the integral. Because of the intimate connection between the resulting formalism and classical mechanics, the illusion is created that in such a way it is possible to avoid the typical problems of quantum mechanics (for example, the ordering problem). It was noted fairly soon that this is not the case.<sup>24, 29, 30</sup> However, appro-

prate rules for taking into account such quantum features encountered in more complicated problems were not adequately developed. Below, this and related questions are discussed, essentially on the basis of Refs. 31-33. As additional literature of review nature devoted to nonrelativistic path integrals, we can mention Refs. 34-47, which can be divided into the clearly mathematical studies of Refs. 34-40 and the physical studies of Refs. 41-47.

The present paper is constructed as follows: In Sec. 1, we discuss Feynman quantization, allowance for nonstandard terms, the equivalence rules, the non-uniqueness of the ordinary expression of the integrals in the Lagrangian formalism, and features of problems with a boundary; the problem of extraterms in the Hamiltonian formalism and associated questions are considered in Sec. 2; Sec. 3 is devoted to canonical transformations of Hamiltonian path integrals; in Sec. 4, we discuss the quantization of dynamical systems with constraints. The concluding remarks are followed by Appendices, which contain some of the lengthy calculations and some auxiliary formulas.

**Notation.** Except where specially stated, we consider a particle of unit mass in  $n$ -dimensional space. We denote the canonical variables by  $q^i, p_i, i = 1, 2, \dots, n$ , and the Poisson brackets by  $\{, \}, \{q, p\} = 1$ . As a rule, we omit the index  $i$ , for example,  $\sum_i q^i p_i = q^i p_i = qp$ . Instead of  $d^n q$  we write  $dq$ ;  $g_{ij}$  and  $g^{ij}$  are, respectively, the covariant and contravariant metric tensors;  $g^{ik} g_{kj} = \delta_j^i, g = \det g_{ij}, \sqrt{g} dq = \bar{d}q$ . We denote functions  $g$  at the points  $q'$  and  $q$  by  $g'$  and  $g$ , respectively. The derivatives with respect to the coordinates are denoted by an index following a comma:  $\partial f / \partial q^i = f_{,i}$ .

Following Dirac,<sup>3</sup> we shall denote by  $|t, q\rangle$  an eigenvector of the operator  $\hat{q}(t)$  with eigenvalue  $q$ . We shall occasionally write the time  $t$  in the form of an index, for example,  $q(t) \equiv q_t, \partial / \partial t \equiv \partial_t, \psi_t(q)$ , etc. As a rule, summation (integration) over repeated indices is understood; for example,  $|q\rangle\langle q| = \int dq |q\rangle\langle q|$ , etc.

## 1. NONSTANDARD TERMS AND EQUIVALENCE RULES. LAGRANGIAN FORMALISM

### Nonstandard terms

We consider a matrix element (kernel) of the evolution operator  $\hat{U}(t - t') = \exp[-i\hat{H}(t - t')/\hbar]$ ; dividing the time interval  $t - t'$  into  $N$  intervals  $\varepsilon = (t - t')/N$ , we represent this kernel in the form<sup>3</sup>

$$\langle q | \hat{U}_{t-t'} | q' \rangle = \int dq_1 \dots dq_{N-1} \langle q | \hat{U}_\varepsilon | q_{N-1} \rangle \dots \langle q_1 | \hat{U}_\varepsilon | q' \rangle. \quad (4)$$

If, following Dirac,<sup>3</sup> we replace  $\langle q_{i+1} | \hat{U}_\varepsilon | q_i \rangle$  by  $\exp[iS(q_{i+1}, q_i)/\hbar]$ , where  $S(q_{i+1}, q_i)$  is the classical action, and go to the limit  $N \rightarrow \infty$ , then apart from an infinite factor we obtain a representation for the propagator in the form of a Feynman path integral,<sup>1</sup> which we shall understand as the limit of the multiple integral (4) and write as

$$\langle q | \hat{U}_{t-t'} | q' \rangle = \int_{q(t')=q'}^{q(t)=q} \mathcal{D}q(t) \exp \left\{ \frac{i}{\hbar} S[q(t)] \right\} \\ \equiv \int \prod_t \frac{dq(t)}{(2\pi i \epsilon \hbar)^{n/2}} \exp \left\{ \frac{i}{\hbar} \int_{t'}^t L dt \right\}. \quad (5)$$

The infinite factor is the limit of  $(2\pi i \epsilon \hbar)^{-nN/2}$  as  $N \rightarrow \infty$ , and it is included in the definition of the measure  $\mathcal{D}q(t)$ . We note that the most important thing for applications is the possibility of treating the repeated integral (4) as a multiple integral, using generalizations of the corresponding prelimit expressions after the passage to the limit. To a large degree, the fruitfulness of the method is associated with this possibility.

For what follows, it is important to note that the matrix elements of the operator  $\hat{U}_\epsilon$  in (4) must be known up to terms of order  $\epsilon$  (the terms of order  $\epsilon^2$  do not contribute to the limit when  $N \rightarrow \infty$ ). The essence of this remark is simple. Since  $\hat{U}_\epsilon \rightarrow \hat{I}$  ( $\hat{I}$  is the identity operator) as  $\epsilon \rightarrow 0$ , the expression (4) is an expression of the type  $(1 + a/N)^N$  with  $N \rightarrow \infty$ , and the terms of order  $1/N^2$  in the round brackets can be ignored. We shall not concern ourselves with the question of the existence of this limit, referring the reader instead to the literature (Refs. 34-40 and 48-53). In all the following calculations, the elementary constituents  $\langle q | \hat{U}_\epsilon | q' \rangle$  in prelimit expressions of the type (4) will be calculated with this accuracy.

Our prescription for obtaining the path integral (5) needs to be made more precise. It is suitable only for Lagrangians of the form

$$L = \dot{q}^2/2 + A\dot{q} - V(q), \quad A = \text{const.} \quad (6)$$

In this case, the elementary factors in the prelimit expression (4) can be expressed as follows ( $\epsilon \rightarrow 0$ ):

$$\langle q_{j+1} | \hat{U}_\epsilon | q_j \rangle = U_{q_{j+1}q_j}(\epsilon) \\ = (2\pi i \hbar)^{-n/2} D^{1/2} \exp \left\{ \frac{i}{\hbar} S(q_{j+1}, q_j) \right\}, \quad (7)$$

where

$$S(q_{j+1}, q_j) = \Delta S \approx \epsilon L \approx \Delta^2/2\epsilon + A\Delta - \epsilon V; \\ D = \det | -\partial^2 S / \partial q_{j+1}^k \partial q_j^l | = \epsilon^{-n}, \quad (8)$$

and  $\Delta = q_{j+1} - q_j$ . Equations (5), (7), and (8) do not hold for Lagrangians of the form

$$L = g_{ij}(q) \dot{q}^i \dot{q}^j / 2 + A_i(q) \dot{q}^i - V(q) \quad (9)$$

(here and in what follows, it is assumed that the functions  $g_{ij}$  and  $A_i$  do not depend on the time). What can we take as a criterion for the validity or invalidity of expressions of the type (5)? The function (5) is the propagator of the particle for  $t > t'$ , i.e., it describes the propagation of the particle and must have the following properties:

1) satisfy the Schrödinger equation

$$i\hbar \partial_t \langle q | \hat{U}_{t-t'} | q' \rangle = \hat{H} \langle q | \hat{U}_{t-t'} | q' \rangle, \quad t - t' > 0, \quad (10)$$

where  $\hat{H}$  is the Hamiltonian acting on the first argument of the kernel;

2) as  $t \rightarrow t'$ , tend to the kernel of the identity operator,

$$\langle q | \hat{U}_{t-t'} | q' \rangle \xrightarrow{t \rightarrow t'} \langle q | q' \rangle; \quad (11)$$

3) ensure fulfillment of the boundary conditions (or conditions equivalent to them).

It will become clear that the function (5) does not satisfy the appropriate Schrödinger equation when the expressions (7)-(9) are used. Condition 3 will be discussed separately (see below).

To find the correct expression for  $\langle q | \hat{U}_\epsilon | q' \rangle$ , we note the following. We have not established the accuracy with which the action in (7) must be calculated. According to Dirac,<sup>3</sup>  $S(q_{j+1}, q_j)$  is the classical action and must be calculated on the true trajectory joining the points  $q_j$  and  $q_{j+1}$ . Feynman<sup>1,2</sup> found that for Lagrangians of the type (6) the classical trajectories in (5) can be approximated by broken lines consisting of segments of straight lines joining the points  $q_j$  and  $q_{j+1}$ . But this prescription may not be correct for more complicated Lagrangians of the type (9), as is in fact the case.<sup>1</sup> Further, the expression (7) for  $\langle q | \hat{U}_\epsilon | q' \rangle$  has the same form as the quasiclassical expansion of a wave function<sup>7,8</sup> and is suitable for generalizations; this suggests that the corresponding function should have this form in the more complicated cases. In Appendix 2, this form of the kernel is justified using different arguments.

Thus, we postulate that in the prelimit expression (4) the elementary factor in the integral (with which we shall basically work in what follows) should be taken to be the expression

$$U_{qq'}(\epsilon) \approx (2\pi i \hbar)^{-n/2} (gg')^{-1/4} D^{1/2} \exp \left\{ \frac{i}{\hbar} S(q, q') \right\}; \\ D = \det \left| -\frac{\partial^2 S}{\partial q^i \partial q'^i} \right|, \quad (12)$$

where  $g = g(q)$ ,  $g' = g(q')$ . The factor  $(gg')^{-1/4}$  always appears with the matrix elements if  $g \neq 1$  (see Appendix 1.1); at the same time, it is necessary to make the substitution  $dq \rightarrow \bar{d}q$  in (4). It is assumed that  $S(q, q')$  is the action and that it is calculated on the true classical trajectory joining the points  $q'$  and  $q$ . The pre-exponential factor must ensure fulfillment of the conditions 1 and 2 and correctly reproduce the corresponding classical picture (see Appendix 2).

We now turn to the question of the accuracy with which  $S(q, q')$  must be calculated. Suppose  $t' = 0$ . To find this action, in the integrand of the Lagrange function

$$S(q, q') = \int_0^\epsilon L(q, \dot{q}) dt; \quad q = q(\epsilon); \quad q' = q(0); \quad \epsilon \rightarrow 0 \quad (13)$$

we must substitute a solution which depends on the initial and final values of the coordinates, i.e.,  $q = q(t, q, q')$ , where  $q(0, q, q') = q'$ ,  $q(\epsilon, q, q') = q$ . The action (13) is calculated in Appendix 3.2. The following expansion of  $S(q, q')$  in powers of  $\Delta = q - q'$  as  $\epsilon \rightarrow 0$  is found:

$$S(q, q') = \frac{1}{2\epsilon} \left[ g_{ij} \Delta^i \Delta^j + \frac{1}{2} g_{ij, k} \Delta^i \Delta^j \Delta^k + \frac{1}{6} \left( g_{ij, kl} - \frac{1}{2} [ij, m] g^{mn} [kl, n] \right) \Delta^i \Delta^j \Delta^k \Delta^l + \dots \right]_{q'} \\ + \left[ A_i \Delta^i + \frac{1}{2} A_{j, i} \Delta^i \Delta^j + \dots + \epsilon V + \dots \right]_{q'} \equiv \tilde{S}(q', \Delta); \quad (14)$$

the  $q'$  appended to the square brackets indicates that all the functions are taken at the point  $q'$ . It is easy to obtain the corresponding expansion of  $S(q, q') \equiv \tilde{S}(q, \Delta)$  in



powers of  $\Delta$  at the point  $q$ . For this, it is sufficient to replace all the functions in (14) by series in powers of  $\Delta$ :  $f(q') = f(q) - \Delta f'(q) + \dots$ . The new expression will differ from the old one in the signs of the terms  $\Delta^3/\varepsilon$  and  $\Delta^2$ . The action (14) is obtained for the real trajectory. Approximation of the trajectories by a straight line  $q(t) = q' + t\Delta/\varepsilon$  also generates extraterms:  $S(q, \Delta) = S_{st}(q, \Delta) + \text{nonstandard terms}$ , where

$$S_{st}(q, \Delta) = g_{ij}(q) \Delta^i \Delta^j / 2\varepsilon - A_i(q) \Delta^i - \varepsilon V(q) \quad (15)$$

(the standard action), but leads to an incorrect Schrödinger equation.

Thus, we must establish what extraterms are to be taken into account and what form the Schrödinger equation then takes. We must also establish how the extraterms are to be handled—when they are present, the prelimit integrals cannot be calculated, since they are not Gaussian.

### Equivalence rules

We shall show that in (14) only the terms that have been written down need to be taken into account and that the obtained action is equivalent to an effective action of standard form, i.e., without extraterms, as in (15). By definition,

$$\psi_\varepsilon(q) \approx \int \bar{d}q' U_{qq'}(q) \psi_0(q'); \quad \bar{d}q = \sqrt{g} dq, \quad (16)$$

where the kernel  $U_{qq'}$  is given by Eqs. (12) and (14), and  $\psi_0 = \psi(q, t')$ ,  $\psi_\varepsilon = \psi(q, t' + \varepsilon)$ . We shall show that to small terms of higher order than  $\varepsilon$ , the function  $U_{qq'}$  in (16) can be replaced by the function  $U_{qq'}^{\text{eff}}$  given by Eq. (7) with  $D = \varepsilon^{-n}$  and  $S$  replaced by  $S^{\text{eff}}$  of the standard form

$$S^{\text{eff}}(q, q') = \frac{1}{2} g_{ij}(q) \frac{\Delta^i \Delta^j}{\varepsilon} - A_i^{\text{eff}}(q) \Delta^i - \varepsilon V^{\text{eff}}(q). \quad (17)$$

Moreover, on the physically realizable functions  $\psi(q)$

$$\int \bar{d}q' (U_{qq'}(q) - U_{qq'}^{\text{eff}}(q)) \psi(q') = O(\varepsilon^2), \quad \varepsilon \rightarrow 0. \quad (18)$$

To prove this, it is sufficient to find the asymptotic behavior of the integral (16) in the limit  $\varepsilon \rightarrow 0$ , and this can be calculated in accordance with Ref. 54 by the method of stationary phase. The point  $q' = q$  makes the main contribution. The following terms of the asymptotic behavior are obtained by expanding all the functions in the integrand [except  $\exp(i g \Delta^2 / 2\varepsilon)$  but including  $\psi_0(q')$ ] in series in powers of  $\Delta$ . After transition to the new variable of integration  $\Delta$ , everything reduces to the calculation of multidimensional Gaussian integrals of products of  $\Delta$ . The corresponding formula is given in Appendix 1 [see §1.2, Eq. (A.16)]; it can be rewritten in the form

$$\int_{-\infty}^{\infty} \frac{d^n \Delta}{(2\pi i \varepsilon \hbar)^{n/2}} \exp\left(\frac{i}{\hbar} g_{ij} \frac{\Delta^i \Delta^j}{2\varepsilon}\right) \{\Delta^{j_1} \dots \Delta^{j_{2k}} - (i\varepsilon \hbar)^k g^{j_1 \dots j_{2k}}\} = 0. \quad (19)$$

Here,  $g^{j_1 \dots j_{2k}}$  denotes the tensor in the square brackets in (A.16). Sometimes, it is helpful to use the generalized formula

$$\int_{-\infty}^{\infty} \frac{d^n \Delta}{(2\pi i \varepsilon \hbar)^{n/2}} \exp\left(\frac{i}{\hbar} g_{ij} \frac{\Delta^i \Delta^j}{2\varepsilon}\right) \times \{\Delta^{j_1} \dots \Delta^{j_{2k}} - (i\varepsilon \hbar)^l \sum g^{j_1 \dots j_{2l}} \Delta^{j_{2l+1}} \dots \Delta^{j_{2k}}\} = 0, \quad (20)$$

in which the sum is taken over the  $(2k-1)!!/(2l-1)!!(2k-2l-1)!!$  permutations of the indices between the sets  $(j_1, \dots, j_{2l})$  and  $(j_{2l+1}, \dots, j_{2k})$  corresponding to the permutations in the identity  $g^{j_1 \dots j_{2k}} = \sum g^{j_1 \dots j_{2l}} g^{j_{2l+1} \dots j_{2k}}$ ,  $l$  is an arbitrary number,  $1 \leq l < k$ . These equations are the basis of the equivalence rules—under the integral sign, the product  $\Delta^{j_1} \dots \Delta^{j_{2k}}$  is equivalent to the tensor  $(i\varepsilon \hbar)^k g^{j_1 \dots j_{2k}}$ ; the product of an odd number of  $\Delta$ 's is obviously equivalent to zero. It is clear from this that in the action it is necessary to take into account the extraterms  $\Delta^3/\varepsilon$ ,  $\Delta^4/\varepsilon$ ,  $\Delta^2$ , and in the factors multiplying the exponential the analogous terms if any are present; in practice, the terms  $\Delta$  and  $\Delta^2$  are encountered. It is clear that in the given class of problems it is also necessary to take into account the terms  $(\Delta^3/\varepsilon)^2$  when expanding the exponential in a series.

We shall find the explicit form of the effective action. The typical integral with which one must deal has the form

$$\bar{\psi}_\varepsilon(q) \approx \int \frac{d^n q' g^{1/2}}{(2\pi i \varepsilon \hbar)^{n/2}} [1 + \alpha_i \Delta^i + \alpha_{ij} \Delta^i \Delta^j] \exp\left[\frac{i}{\hbar} S(q, \Delta)\right] \psi_0(q'); \quad (21)$$

$$S(q, \Delta) = g_{ij} \frac{\Delta^i \Delta^j}{2\varepsilon} + B_{ijk} \frac{\Delta^i \Delta^j \Delta^k}{\varepsilon} + C_{ijkl} \frac{\Delta^i \Delta^j \Delta^k \Delta^l}{\varepsilon} + A_i \Delta^i + D_{ij} \Delta^i \Delta^j - \varepsilon V, \quad (22)$$

where in our particular case [the Lagrangian (9) and the action (14) expanded in the neighborhood of the point  $q$ ]

$$B_{ijk} = -g_{ij,k}/4; \quad C_{ijkl} = (g_{ij,kl} - \frac{1}{2}[ij, m] g^{mn} [kl, n]) / 6; \quad D_{ij} = -A_{j,i}/2. \quad (23)$$

The terms in the square brackets in (21) may derive from the expansion of the pre-exponential factor in (12) or the function  $g'^{1/2}$  in powers of  $\Delta$ ; in the latter case,

$$\alpha_i = -g^{ij} g_{jk,i} / 2; \quad \alpha_{ij} = \{g_{hl,i} g_{mn,j} / 2 - g_{lm,i} g_{jn,j} / 2\} g^{hl} g^{mn} + g^{mn} g_{mn,ij} / 4. \quad (24)$$

It is assumed that  $\psi(q')$  in (21) is also expanded in a series:  $\psi(q) - \Delta^i \partial_i \psi(q) + \dots$

Transforming the integral (21), it is helpful to bear in mind the following proposition: The terms even in  $\Delta$  (apart from the main term  $\Delta^2/\varepsilon$ ) in the exponential or multiplying it can be replaced by the terms equivalent to them in accordance with (19) at any stage of the calculations. Indeed, it is readily seen that any power of terms even in  $\Delta$ , like products of them or combinations of them with odd terms, makes a contribution of order  $\varepsilon^2$ . Therefore, even terms can be replaced by the equivalent terms directly in the exponential, and terms multiplying the exponential can be taken into its argument. Applying this rule to the even terms in (21), we find that the potential is augmented by the terms

$$\hbar^2 C_{ijkl} g^{ijkl} - i \hbar D_{ij} g^{ij} - \hbar^2 \alpha_{ij} g^{ij}. \quad (25)$$

In (21), only odd terms remain. The square  $(i\hbar)^2 (B \Delta^3/\varepsilon + A \Delta)^2 / 2$  of odd terms which arises when the exponential is expanded also contains only even terms, so that the potential is augmented by the further term

$$[-\hbar^2 B_{ijk} \tilde{B}^{ijk} + 2i\hbar A_i \tilde{B}^i + A_i A^i] / 2, \quad (26)$$

where

$$\tilde{B}^{ijk} = B_{lmn} g^{ijklmn}; \quad \tilde{B}^i = B_{ijh} g^{ijhl}; \quad A^i = A_j g^{ij}. \quad (27)$$



Finally, the product of  $\alpha\Delta$  and odd terms from the exponential makes the contribution

$$\alpha_i (\hbar^2 \tilde{B}^i - i\hbar A^i) \quad (28)$$

to the potential.

There remains only a sum of odd terms, which is combined with  $-\Delta^i \partial_i \psi$ :

$$-\left[ \alpha_i \Delta^i + \frac{i}{\hbar} \left( B_{ijh} \frac{\Delta^i \Delta^j \Delta^h}{\varepsilon} + A_i \Delta^i \right) \right] \Delta^i \partial_i \psi. \quad (29)$$

The terms containing the fourth power of  $\Delta$  can be transformed by means of (20) into quadratic terms:

$$B_{ijh} \frac{\Delta^i \Delta^j \Delta^h \Delta^i}{\varepsilon} \rightarrow i\hbar B_{(ijk)} g^{ij} \Delta^h \Delta^i; \quad B_{(ijk)} = B_{ijh} + B_{jhi} + B_{kij}. \quad (30)$$

Using this substitution in (29), we can achieve linearity in  $\Delta$  of the coefficient of  $\Delta^i \partial_i \psi$ . The transformed sum in the square brackets in (29) can now be taken into the argument of the exponential. It is only necessary to bear in mind that when the resulting exponential is expanded in a series it is necessary to take into account the square of the linear terms, i.e., to the potential it is necessary to add a term that compensates this square:

$$-\beta_i \beta_j g^{ij}/2; \quad \beta_j = A_j + i\hbar (B_{(ijk)} g^{ik} - \alpha_j). \quad (31)$$

Collecting all the terms included in the potential and using (29), (30), and (27), we find that in the effective action (17)

$$\left. \begin{aligned} A_j^{\text{eff}} &= A_j + i\hbar (\tilde{B}_j - \alpha_j); \\ V^{\text{eff}} &= V + \hbar^2 [C_{ijkl} g^{ijkl} - B_{ijk} B^{ijk} + (\alpha_i \alpha_j / 2 - \alpha_{ij}) g^{ij}] - i\hbar D_{ij} g^{ij}. \end{aligned} \right\} \quad (32)$$

Since the odd powers of  $\Delta$  are equivalent to zero, the terms omitted in the derivation have the order  $\varepsilon^2$ . This proves the proposition (18). Equations (17) and (32) are the content of the equivalence rules for an action with extraterms of general form [as in (21) and (22)]. Using the relation (19) again, it is not difficult to show that the function  $\psi_\varepsilon(q)$  (21) satisfied the equation

$$i\hbar \partial_\varepsilon \bar{\psi}_\varepsilon = [-\hbar^2 g^{ij} \partial_i \partial_j / 2 + i\hbar g^{ij} A_i^{\text{eff}} \partial_j + g^{ij} A_i^{\text{eff}} A_j^{\text{eff}} / 2 + V^{\text{eff}}] \bar{\psi}_\varepsilon. \quad (33)$$

If the tensors which occur in (22) are defined by Eqs. (23) and (24), then, substituting these expressions in (33) and making the substitution  $\varepsilon \rightarrow t$ , we find

$$i\hbar \partial_t \bar{\psi}_t = (\hat{H} + \hbar^2 R/6) \bar{\psi}_t, \quad (34)$$

where  $\hat{H}$  is given by Eq. (A.32);  $R$  is the scalar curvature (A.11).

Hitherto, we have ignored the factor  $(gg')^{-1/4} D^{1/2}$  in front of the exponential (12). As is shown in Appendix 3.3,

$$D = [(gg')^{1/2}/\varepsilon^n] (1 + R_{ij} \Delta^i \Delta^j / 6), \quad (35)$$

i.e., allowance for this factor leads only to the modification  $\alpha_{ij} \rightarrow \alpha_{ij} + R_{ij}/12$  of the tensor  $\alpha_{ij}$ , and in accordance with (32) this means that the term  $-\hbar^2 R/12$  is added to the potential. Then the second term on the right-hand side of (34) is replaced by  $\hbar^2 R/12$ . The same equation will be satisfied by the kernel (12) with the action (14) in the limit  $t \rightarrow 0$ :

$$i\hbar \partial_t U_{qq'}(t) = (\hat{H} + \hbar^2 R/12) U_{qq'}(t) \quad (36)$$

( $\hat{H}$  acts on the first argument of the kernel). The obtained equation is identical to (A.33). There are two striking things here. First, we have obtained a correct expression for  $\hat{H}$  with allowance for the order in which the operators follow each other. This is the form that the Hamiltonian takes after transition from Cartesian to curvilinear coordinates. Second, a term proportional to  $\hbar^2$  has appeared; it is absent in the classical Hamiltonian and disappears on the transition to flat space. These features of Eq. (36) are discussed in Sec. 5.

We note that the presence in (21) of a  $q'$ -dependent pre-exponential factor [for example,  $\gamma(q')$ ] does not alter our conclusion—the factor can be taken into  $\psi_0(q')$  for the time being. It is easy to go over from  $\gamma(q')$  to  $\gamma(q)$ ; this leads merely to a redefinition of the standard action. Suppose  $\gamma(q') = \gamma(q)(1 + \gamma_i \Delta^i + \gamma_{ij} \Delta^i \Delta^j)$ ; then, using the formula

$$1 + \gamma_i \Delta^i + \gamma_{ij} \Delta^i \Delta^j = \exp[\gamma_i \Delta^i + (\gamma_{ij} - \gamma_i \gamma_j / 2) \Delta^i \Delta^j] + O(\Delta^3) \quad (37)$$

and the rule (19), we find that the entire change in  $S^{\text{eff}}$  reduces to the substitutions

$$A_i^{\text{eff}} \rightarrow A_i^{\text{eff}} - i\hbar \gamma_i; \quad V^{\text{eff}} \rightarrow V^{\text{eff}} - \hbar^2 (\gamma_i \gamma_j / 2 - \gamma_{ij}) g^{ij}. \quad (38)$$

The fact that  $\gamma_i$  and  $\gamma_{ij}$  [or  $\alpha_i$  and  $\alpha_{ij}$  in (32)] are not contracted with the remaining tensors is what makes it possible to use (32) independently of the argument of the pre-exponential factor.

### Nonuniqueness of the formal expression (5)

Extraterms are encountered not only on quantization of classical systems with Lagrange functions of the type (9). They also appear as a result of nonlinear coordinate transformations, and one must reckon with them when the limit of (4) is expressed in the form (5). We shall now discuss these questions in more detail.

We begin by considering the meaning contained in the formal expression (5). After transition to the effective action (17), the argument of the exponential in (5) can be written in the form of an integral with respect to the time of an effective Lagrangian:

$$S(q, q') = \int_{q'}^q L^{\text{eff}}(q, \dot{q}) dt; \quad L^{\text{eff}} = g_{ij}(q) \dot{q}^i \dot{q}^j / 2 + A_i^{\text{eff}}(q) \dot{q}^i - V^{\text{eff}}(q). \quad (39)$$

This expression is obviously ambiguous and does not contain a unique rule for calculating the integral. The point is that the path integral (5) is defined as the limit of (4). But in accordance with (5) and (39) it is impossible to recover uniquely the prelimit expression (4). The recovered infinitesimal action will have the form (17), and the functions  $g_{ij}$  and  $A_i^{\text{eff}}$  can be taken at any point of the interval  $[q, q']$ , i.e.,  $q_\alpha = q - \alpha(q - q')$ ,  $0 \leq \alpha \leq 1$ , can be taken as their argument. When  $\alpha=0$ , this will be the point  $q$ , and when  $\alpha=1$  the point  $q'$ ; taking  $\alpha=1/2$ , we obtain  $(q + q')/2$ . In the case of the usual expression, any choice of  $\alpha$  in the limit  $N \rightarrow \infty$  gives formally the same expression for the integrals (5) and (39), but the corresponding limits of the expression (4) after substitution in it of the expression (12) will be different. They will depend on  $\alpha$ , since now the action depends on  $\alpha$ :  $S_\alpha(q, q') \equiv S(q_\alpha, \Delta)$ . Indeed, if all the functions in (17) are taken, for example, at the points  $q_\alpha$  or

$q_\beta$ , then it follows by virtue of the equation  $q_\alpha = q_\beta - (\alpha - \beta)\Delta$  that the terms

$$S_\alpha - S_\beta = -\frac{(\alpha - \beta)}{2} g_{ij, h} (q_\beta) \frac{\Delta^i \Delta^j \Delta^h}{\varepsilon} + \frac{(\alpha - \beta)^2}{4} g_{ij, kl} (q_\beta) \frac{\Delta^i \Delta^j \Delta^k \Delta^l}{\varepsilon} - (\alpha - \beta) A_{i, j}^{\text{eff}} \Delta^i \Delta^j, \quad (40)$$

which cannot be ignored. All this recalls the situation with the ordering of noncommuting operators in a Hamiltonian. In Sec. 2, we shall see that there is indeed a connection here.

Thus, the ordinary formal expression of the path integral in the form (5) is incompletely defined in the case of Lagrangians of the form (9). It is necessary to specify the point at which the functions are taken in the reconstruction of the prelimit expressions (4), using, for example, the symbol  $\alpha$  in the integral

$$\int (\alpha) \mathcal{D}q(t) \exp \left( -\frac{i}{\hbar} S \right), \quad (41)$$

or in the action (Lagrangian, function multiplying the exponential). It is obvious that the arguments of the functions in the different subintervals  $\Delta t_i = \varepsilon$  of the time interval can be chosen arbitrarily, i.e.,  $\alpha$  in (41) can be a function of the time. This gives the formalism a certain flexibility; for example, it becomes possible to differentiate (variationally) with respect to  $\alpha(t)$ .

We note in conclusion that a path integral with index  $\alpha$  can always be expressed as an integral with any other index but with an appropriately modified action. Using the connection between  $q_\alpha$  and  $q_\beta$ , all the functions in the standard infinitesimal action can be expanded in powers of  $(\alpha - \beta)\Delta$  in the neighborhood of  $q_\beta$ , the extraterms [for the Lagrangian (39), they are given by Eq. (40)] being retained. The extraterms can be eliminated by means of the equivalence rules (one can show that they are valid for any  $q_\alpha$ ) by noting that by virtue of (40)

$$B_{ijh} = -\frac{\alpha - \beta}{2} g_{ij, h} (q_\beta); \quad C_{ijh} = \frac{(\alpha - \beta)^2}{4} g_{ij, kl} (q_\beta); \quad D_{ij} = -(\alpha - \beta) A_{i, j}^{\text{eff}} (q_\beta), \quad (42)$$

and by going over to new effective potentials  $A_i$  and  $V$  in accordance with (32). In this way, we prove the formula

$$\int \mathcal{D}q(t) \exp \left( -\frac{i}{\hbar} S_\alpha \right) = \int \mathcal{D}q(t) \exp \left( -\frac{i}{\hbar} S_\beta^{\text{eff}} \right), \quad (43)$$

where  $S_\beta^{\text{eff}}$  for an infinitesimally small time interval  $\varepsilon$  is

$$S_\beta^{\text{eff}}(q_\beta, \Delta) = S_\beta - i\hbar \tilde{B}_i(q_\beta) \Delta^i - \varepsilon \{ \hbar^2 [C_{ijh} g^{ijhl} - B_{ijh} B^{(ij)h}] - i\hbar D_{ij} g^{ij} \}; \quad (44)$$

$S_\beta$  is obtained from  $S_\alpha$  by the substitution  $q_\alpha \rightarrow q_\beta$  and the tensors  $B, C$ , etc., are defined by Eqs. (27), (30), and (42). In (43), we have not taken into account the weight factors multiplying the exponential; they must also carry an index (the arguments of the functions in the exponential and multiplying the exponential need not be the same). In accordance with (37) and (38), the change  $\alpha \rightarrow \beta$  of the index of the pre-exponential factor  $\gamma_\alpha \equiv \gamma(q_\alpha)$  changes  $S_\beta^{\text{eff}}$  in (43):

$$S_\beta^{\text{eff}} \rightarrow S_\beta^{\text{eff}} + i\hbar (\alpha - \beta) (\ln \gamma_\beta)_{, j} \Delta^j + \varepsilon \frac{\hbar^2}{2} (\alpha - \beta)^2 g^{ij} (\ln \gamma_\beta)_{, ij}.$$

#### Allowance for boundary conditions

Hitherto, we have considered problems in a space without a boundary, in which the natural requirement of

decrease of the wave function at infinity followed automatically from the general formula (5) [or from (16)]. One not infrequently encounters problems in which there is a boundary at a finite distance. An example is the already mentioned problem of a particle in a box.<sup>4,55</sup> Similar problems arise as a result of coordinate transformation (transition to angle variables), in the study of dynamics on a group,<sup>13-15</sup> and in chiral theories. In these cases, direct application of the standard scheme of Ref. 1 does not achieve the goal. The reason for the failure is obvious—the solution must satisfy appropriate boundary conditions, whereas the formalism considered above guarantees only that the solution decreases at infinity. Since the Green's function must ensure fulfillment of the boundary conditions, the expressions given above must be suitably modified.

To clarify the difficulties that then arise, we consider a very simple example: a particle of unit mass in a one-dimensional box of length  $L$ ; let the points 0 and  $L$  be the "walls" of the box. It is incorrect to express the kernel of the evolution operator in the form

$$\langle q | \hat{U}_t | q' \rangle = \lim_{N \rightarrow \infty} (2\pi i \varepsilon \hbar)^{-1/2} \int_0^L \dots \int_0^L \prod_{j=1}^{N-1} \frac{dq_j}{(2\pi i \varepsilon \hbar)^{1/2}} \exp \left\{ \frac{i}{\hbar} \sum_{j=0}^{N-1} \frac{(q_{j+1} - q_j)^2}{2\varepsilon} \right\} \quad (45)$$

(where  $\varepsilon = t/N$ ,  $q_N = q$ ,  $q_0 = q'$ ), since even for  $t = \varepsilon$ ,  $\varepsilon \rightarrow 0$ , the wave function

$$\begin{aligned} \psi_\varepsilon(q) &\approx \int_0^L \frac{dq'}{(2\pi i \varepsilon \hbar)^{1/2}} \exp \left[ \frac{i}{\hbar} \frac{(q - q')^2}{2\varepsilon} \right] \psi_0(q') \\ &\equiv \int_0^L U_\varepsilon(q - q') \psi_0(q') dq' \end{aligned} \quad (46)$$

satisfies the Schrödinger equation for  $0 < q < L$  but not the boundary conditions  $\psi_\varepsilon(0) = \psi_\varepsilon(L) = 0$  [even if  $\psi_0(0) = \psi_0(L) = 0$ ]. Therefore, (45) does not solve the problem. Moreover, the integral (45) cannot be calculated explicitly, despite the simplicity of the integrand (Gaussian exponential).

The correct procedure was already pointed out by Pauli.<sup>4</sup> The function (45) satisfies the Schrödinger equation, and it is therefore necessary to take several such solutions and combine them in order to satisfy the conditions at the boundary. As a result, "using the method of images" (Pauli), we find that in the integrand of (46) we must replace  $U_\varepsilon$  by the function

$$K'(q, q'; \varepsilon) = \sum_{n=-\infty}^{\infty} [U_\varepsilon(q - q' + 2Ln) - U_\varepsilon(q + q' + 2Ln)]. \quad (47)$$

It is easy to show that  $K'$  (for all times  $t > 0$ ) is the Green's function of the problem

$$K(q, q'; t) = \sum_{n=1}^{\infty} \psi_n(q) \psi_n^*(q') \exp(-iE_n t/\hbar), \quad t > 0, \quad (48)$$

where  $\psi_n(q) = (2/L)^{1/2} \sin(\pi n q/L)$ ,  $E_n = \pi^2 \hbar^2 n^2 / 2L^2$ . The solution has been found, but the transition to the path integral involves the disagreeable necessity of integrating Gaussian exponentials (the kernels  $K'$ ) between finite limits. Equation (46) with the kernel (47) can be rewritten in the form



$$\psi_\varepsilon(q) \approx \sum_{n=-\infty}^{\infty} \left\{ \int_{2Ln}^{L+2Ln} dq' U_\varepsilon(q-q') \psi_0(q'-2Ln) - \int_{2Ln-L}^{2Ln} dq' U_\varepsilon(q-q') \psi_0(-q'+2Ln) \right\}. \quad (49)$$

On the real axis, we define the function  $\Psi_0(\Psi_0 = \psi_0(q)$  if  $q \in [0, L]$ ):

$$\Psi_0(-q) = -\Psi_0(q); \Psi_0(q+2Ln) = \Psi_0(q); \Psi_0(0) = \Psi_0(L) = 0. \quad (49a)$$

By means of it, we rewrite (49) as

$$\psi_\varepsilon(q) \approx \int_{-\infty}^{\infty} dq' U_\varepsilon(q-q') \Psi_0(q'). \quad (50)$$

It is readily verified that the function  $\psi_\varepsilon(50)$  satisfies the conditions (49a) and the Schrödinger equation. In the path integral, we can therefore now integrate over the complete real axis but apply the obtained kernel to the function  $\Psi_0$ , which is defined in the whole of space and is constructed from the function  $\psi_0$  (in the given case as an odd,  $2L$ -periodic function). The problem is solved. The kernel  $U_\varepsilon(q-q')$  can be represented in the form of the path integral (45), in which the integration is within infinite limits. Application of it to the function  $\Psi_0$  gives the required result.

Thus, there are two possibilities: 1) the Green's function of the problem (47) can be used and the integration is performed with finite limits; 2) the kernel  $U_\varepsilon(q-q')$  can be used and the integration is with infinite limits. In the second case,  $U_\varepsilon(q-q')$  must be applied to the function  $\Psi_0$  constructed using the initial value  $\psi_0$  and defined in accordance with (49a) in the whole of space.

We shall establish the general structure of the solution for a number of problems of this type.<sup>56</sup> Let  $\hat{H} = -\hbar^2 \Delta/2 + V$  be the Hamiltonian describing the motion of a particle in  $n$ -dimensional Euclidean space, and let the potential  $V(q)$  be an analytic function with respect to each variable  $q^i$  in the neighborhood of the entire real axis; we denote by  $\Gamma$  the boundary of the region of motion  $\Omega$ . We shall assume that the boundary is sufficiently smooth and (to be specific) that the volume of the region  $\Omega$  is bounded. Suppose  $U(q, q'; t)$  is given by Eq. (5), in which  $t' = 0$ ,  $L = \dot{q}^2/2 - V$ , and the integration over  $q$  is with infinite limits. Then in accordance with the possibilities 1) and 2) we must know how to construct either the Green's function  $K(q, q'; t)$  or the function  $\Psi_0(q)$ . The solutions are given by

$$K(q, q'; t) = \int_{-\infty}^{\infty} U(q, q''; t) Q(q'', q') dq'', t > 0; \quad (51)$$

$$\Psi_0(q) = \int_{q' \in \Omega} Q(q, q') \Psi_0(q') dq', \quad (52)$$

where

$$Q(q, q') = \sum_{(k)} \psi_{(k)}(q) \psi_{(k)}^*(q'), \quad (53)$$

in which  $\psi_{(k)}(q)$  is a complete orthonormal set of eigenfunctions of  $\hat{H}$ ,  $\hat{H}\psi_{(k)} = E_{(k)}\psi_{(k)}$ , satisfying the boundary conditions

$$\psi_{(k)}(q)|_{\Gamma} = 0; \quad (54)$$

here,  $(k)$  denotes the complete set of quantum numbers that characterize the vectors  $\psi_{(k)}$ . By virtue of the an-

alyticity of the potential, the functions  $\psi_{(k)}(q)$  can be continued analytically beyond the region  $\Omega$ , this defining  $Q(q, q')$  and  $\Psi_0(q)$  for all values of  $q$ .

Note that for  $q, q' \in \Omega$ ,  $Q(q, q')$  is simply the  $\delta$  function. But if  $q \notin \Omega$ , then  $Q$  is a continuation of the  $\delta$  function beyond  $\Omega$  that is natural for the given problem. It is easy to prove these propositions. Using the formula (see Refs. 1 and 2 and also Sec. 2)

$$\int_{-\infty}^{\infty} U(q, q'; \varepsilon) \Psi_0(q') dq' \approx \left(1 - \frac{i\varepsilon}{\hbar} \hat{H}\right) \Psi_0(q), \varepsilon \rightarrow 0, \quad (55)$$

and using (53), we obtain for (51)

$$K(q, q'; \varepsilon) \approx \left(1 - \frac{i\varepsilon}{\hbar} \hat{H}\right) Q(q, q') \approx \sum_{(k)} \exp\left(-\frac{i\varepsilon E_{(k)}}{\hbar}\right) \psi_{(k)}(q) \psi_{(k)}^*(q'), \quad (56)$$

from which it follows that  $K(q, q'; t)$  is indeed the Green's function of the problem: It obviously satisfies the Schrödinger equation and the boundary conditions [by virtue of (54)] and tends to the  $\delta$  function as  $t \rightarrow 0$ . The need for integration in (51) within infinite limits was required on the transition from this formula to the first equation in (56). In concrete applications of this scheme, it is necessary to establish convergence of the employed integrals, or rather, the possibility of giving them meaning. In fact, this can be readily done for integrals of the type (50) with kernel (46) even for functions  $\Psi_0$  that increase fairly rapidly (for example, as a Gaussian exponential) at infinity (the function  $\Psi_0$  is normalized in the physical region). In Ref. 56, the expressions we have found were used to solve the problem of a particle within a disk. In this case, all the calculations can be performed explicitly.

In quantum mechanics, one encounters problems in which the coordinate varies in a finite range and one merely imposes on the wave function the condition of periodicity, i.e., the wave function is not required to vanish at the ends of the interval. In this case, only periodicity is required of the Green's function  $K$ . Then if the function  $U(q, q'; t)$  satisfies the Schrödinger equation and has the property  $U(q+nL, q'; t) = U(q, q'-nL, t)$ , and  $U(q, q'; t) \rightarrow \delta(q-q'), t \rightarrow 0$ , then  $K$  is given by the sum

$$K(q, q'; t) = \sum_{n=-\infty}^{\infty} U(q+nL, q'; t) = \sum_{n=-\infty}^{\infty} U(q, q'-nL; t), \quad (57)$$

i.e.,

$$\psi_t(q) = \int_0^L dq' K(q, q'; t) \psi_0(q') \quad (58)$$

is the solution of the problem  $[\psi_t(q+nL) = \psi_t(q)]$ . Since  $\psi_0(q)$  is a periodic function, we can, using (57), write Eq. (58) in the form

$$\psi_t(q) = \int_{-\infty}^{\infty} dq' U(q, q'; t) \psi_0(q'). \quad (59)$$

which is suitable for transition to a path integral.

The significance of the appearance of the sums or differences in (47) and (57) is simple. In (47) there are, besides the straight line joining the points  $q$  and  $q'$ , extremal paths that touch the boundary (reflected paths).

By virtue of the vanishing required by the boundary condition, they must not contribute, and therefore compensating terms are subtracted. In contrast, allowance is made for the fact in (57) that besides the straight (shortest) line joining the points  $q$  and  $q'$  there are extremal paths that differ by  $nL$  (which pass, for example,  $n$  times round a circle), whose contribution cannot be ignored. The expression (57) is used below. An exterior problem (a particle outside a convex region) is briefly discussed in Ref. 20.

### Change of variables

It is now almost obvious that extraterms will also be encountered when nonlinear changes of variables are made in a Lagrangian path integral. Since the infinitesimal action of the standard form (15) depends on the coordinate difference  $\Delta = q - q'$ , the differences  $\Delta^i$  are replaced on the transition to the new variables  $q^i = q^i(Q)$  by part of a series ( $\Delta_Q = Q - Q'$ ):

$$\Delta^i = q^i(Q) - q^i(Q') = q^i_{,j}(Q) \Delta Q^j - \frac{1}{2} q^i_{,jk}(Q) \Delta Q^j \Delta Q^k + \frac{1}{6} q^i_{,jkl}(Q) \Delta Q^j \Delta Q^k \Delta Q^l - \dots \quad (60)$$

All the terms that have been written down (see above) must be taken into account [ $\Delta_Q^3$  makes a contribution  $\sim \Delta^4/\varepsilon$  when (60) is substituted in the first term of (15)].

We introduce the following notation. Let  $d$  be the matrix with elements  $d^i_j = q^i_{,j}(Q)$ . We define

$$c^i_{jk} = -(d^{-1})^i_l q^l_{,jk}(Q)/2; \quad c^i_{jhl} = \frac{1}{6} (d^{-1})^i_l q^l_{,jhl}(Q), \quad (61)$$

where  $d^{-1}$  is the inverse matrix. In the new notation,

$$\Delta^i = d^i_j (\Delta Q^j + c^j_{jk} \Delta Q^k + c^j_{jhl} \Delta Q^k \Delta Q^l + \dots). \quad (62)$$

Substituting (62) in the action (15), we find that it has the same structure as the expression (22), in which  $g_{ij} \rightarrow \tilde{g}_{ij}$ ,  $A_i \rightarrow \tilde{A}_i$  and the tensors  $\tilde{g}_{ij}$ ,  $\tilde{A}_i$ ,  $B_{ijk}$ , etc., are expressed in terms of the tensors  $d^i_j$ ,  $c^i_{jk}$ , ...:

$$\left. \begin{aligned} \tilde{g}_{ij}(Q) &= g_{ij}(q(Q)) d^i_l d^j_l; \quad B_{ijk} = \tilde{g}_{il} c^l_{jk}; \\ C_{ijkl} &= \tilde{g}_{il} c^l_{jkh} + \tilde{g}_{jl} c^l_{ikh} + \tilde{g}_{kl} c^l_{ijh} / 2; \quad \tilde{A}_i = d^j_i A_j; \quad D_{ij} = \tilde{A}_i c^k_{jk}. \end{aligned} \right\} \quad (63)$$

We can now use the general expression (32). After some calculations, we obtain the following result:  $S^{\text{eff}}$  is given by Eq. (17), in which  $g_{ij}$  must be replaced by  $\tilde{g}_{ij}$ , and  $A_j^{\text{eff}}$  and  $V^{\text{eff}}$  are taken to be

$$\left. \begin{aligned} A_j^{\text{eff}} &= A_j + i\hbar (\tilde{g}_{jl} c^k_{jk} + 2c^k_{jhl}); \\ V^{\text{eff}} &= V + \hbar^2 [3c^i_{jkh} c^j_{ij} c^k_{kh} / 2 - 2c^i_{ij} c^k_{ij}] + \frac{i\hbar}{2} A_k q^k_{,jj}. \end{aligned} \right\} \quad (64)$$

The summation over repeated subscripts (or superscripts) is performed by means of the tensor  $\tilde{g}^{ij}$  (respectively,  $\tilde{g}_{ij}$ ); for example,  $c^i_{kk} = c^i_{kh} \tilde{g}^{kh}$ . We then arrive at the required rule for transforming the expression (16) when the change of variables is made:

$$\begin{aligned} \psi_e &\approx \int \frac{V \tilde{g}' dq'}{(2\pi i \varepsilon \hbar)^{n/2}} \exp \left[ \frac{i}{\hbar} S_0(q, q') \right] \psi_0(q') \\ &= \int \frac{V \tilde{g}' dQ'}{(2\pi i \varepsilon \hbar)^{n/2}} \exp \left[ \frac{i}{\hbar} S_0^{\text{eff}}(Q, Q') \right] \psi_0(q(Q')). \end{aligned} \quad (65)$$

Here,  $\tilde{g}' = g' J^2(Q')$ , where  $J = \det q^i_{,j}$  (Jacobian of the transformation); it is assumed that  $S_0$  has the standard form (15) and is taken at the point  $q$ , i.e.,  $\alpha=0$ , and  $S_0^{\text{eff}}$  is given by Eqs. (17) and (64) (in the first,  $g_{ij} \rightarrow \tilde{g}_{ij}$ ). For Lagrangians of the special form  $L = \dot{q}^2/2 - V$ , a cor-

responding  $S^{\text{eff}}$  was obtained in Ref. 11.

*Example.* We consider the transition to polar coordinates in the problem of a free particle in two-dimensional space. We have ( $\Delta_\varphi = \varphi - \varphi'$ ):

$$\begin{aligned} &\frac{1}{2\pi i \hbar} \exp \left[ \frac{i}{\hbar} \frac{(x-x')^2}{2t} \right] \\ &= \frac{1}{2\pi i \hbar} \left[ \frac{i}{2\hbar} (r^2 + r'^2 - 2rr' \cos \Delta_\varphi) \right] = K(r, r', \Delta_\varphi; t); \end{aligned} \quad (66)$$

as assumed, the Green's function has the periodicity property  $K(r, r', \Delta_\varphi + 2\pi n; t) = K(r, r', \Delta_\varphi; t)$ . But in constructing the path integral, we use only the asymptotic behavior of  $K$  as  $t \rightarrow 0$ , which is determined by the critical points of the argument of the exponential, i.e., by the solutions of the equations  $\sin \Delta_\varphi = 0$ ,  $r - r' \cos \Delta_\varphi = 0$ :  $\Delta_\varphi = 0, \pi$  (or  $-\pi$ , making the solution  $\varphi'_0$  lie in the interval  $[0, 2\pi]$ ) and accordingly  $r'_0 = \pm r$ . Therefore, restricting ourselves to the first few terms in the expansion of the argument of the exponential in the neighborhood of the critical points, we arrive at a representation for the Green's function  $K$  ( $t \rightarrow 0$ ,  $\Delta_r = r - r'$ ):

$$K_{\text{as}} = \frac{1}{2\pi i \varepsilon \hbar} \left\{ \exp \left[ \frac{i}{2\varepsilon \hbar} \left( \Delta_r^2 + rr' \left( \Delta_\varphi^2 - \frac{\Delta_\varphi^4}{12} \right) \right) \right] + \left( \begin{matrix} r' \rightarrow -r' \\ \varphi' \rightarrow \varphi' + \pi \end{matrix} \right) \right\} \quad (67)$$

(only the important extraterms have been written out). However,  $K_{\text{as}}$  does not have the property of periodicity with respect to  $\varphi$ , i.e.,  $K_{\text{as}}$  is not the Green's function of the problem. In accordance with (57), the correct expression for  $K$  is given by

$$K_e = \sum_{n=-\infty}^{\infty} K_{\text{as}}(r, r', \Delta_\varphi + 2\pi n; \varepsilon). \quad (68)$$

Using (68), we can write the expression for the time-shifted function in the form

$$\begin{aligned} \psi_e(r, \varphi) &\approx \int_0^\infty \int_0^{2\pi} r' dr' d\varphi' K_e(r, r', \Delta_\varphi) \psi_0(r', \varphi') \\ &= \int_{-\infty}^\infty \int_{-\infty}^\infty \frac{r' dr' d\varphi'}{2\pi i \varepsilon \hbar} \exp \left\{ \frac{i}{2\varepsilon \hbar} \left[ \Delta_r^2 + rr' \left( \Delta_\varphi^2 - \frac{\Delta_\varphi^4}{12} \right) \right] \right\} \psi_0(r', \varphi'), \end{aligned} \quad (69)$$

where the function  $\psi_0$  is defined in the complete space [ $\psi_0$  is a function periodic in  $\varphi'$  and  $\psi_0(-r, \varphi) = \psi_0(r, \varphi + \pi)$ , with  $\psi_0 = \psi_0$  in the physical region]. Using the rule (64)–(65) for the change of variables, we can rewrite this expression as

$$\psi_e \approx \int_{-\infty}^\infty \int_{-\infty}^\infty \frac{V \tilde{g}' dr' d\varphi'}{2\pi i \varepsilon \hbar} \exp \left\{ \frac{i}{\hbar} \left[ \frac{\Delta_r^2}{2\varepsilon} + \frac{r^2 \Delta_\varphi^2}{2\varepsilon} + \varepsilon \frac{\hbar^2}{8r^2} \right] \right\} \psi_0(r', \varphi'). \quad (70)$$

It follows directly from this that  $\psi_e$  satisfies the Schrödinger equation and is defined in the unphysical region in the same way as  $\psi_0$ , i.e., transition to the path integral is admissible. The correctness of this expression is confirmed by the calculations in Appendix 4.1, in which it is obtained by other arguments [without using (57)]. It follows from (70) that in the obtained path integral it is necessary to integrate over  $r$  and  $\varphi$  with infinite limits.

## 2. NONSTANDARD TERMS AND EQUIVALENCE RULES. HAMILTONIAN FORMALISM

### Hamiltonian path integral and nonstandard terms

A Hamiltonian path integral can also be obtained from (4) by substituting the following integral representation



for  $\mathbf{U}_{qq}(\varepsilon)$ :

$$\begin{aligned} \langle q | \hat{\mathbf{U}}(\varepsilon) | q' \rangle &= \langle q | \exp \left( -\frac{i\varepsilon}{\hbar} \hat{H} \right) | q' \rangle \\ &\approx \langle q | 1 - \frac{i\varepsilon}{\hbar} H(\hat{q}, \hat{p}) | q' \rangle = \langle q | 1 - \frac{i\varepsilon}{\hbar} H(q, p) | p \rangle \langle p | q' \rangle \\ &\approx \int dp \exp \left[ -\frac{i\varepsilon}{\hbar} H(q, p) \right] \langle q | p \rangle \langle p | q' \rangle. \end{aligned} \quad (71)$$

Here, we have used the equation

$$\langle q | H(\hat{q}, \hat{p}) | p \rangle = H(q, p) \langle q | p \rangle; \quad (72)$$

and, in addition, in the second and last stages of the derivation we have ignored terms of order  $\varepsilon^2$  [it is assumed that they make no contribution when we go to the limit  $N \rightarrow \infty$  in (4)]. If the determinant  $g$  of the metric tensor is equal to unity, then, bearing in mind that  $\langle q | p \rangle = (2\pi\hbar)^{-n/2} \exp(ipq/\hbar)$ , we obtain

$$\langle q | \hat{\mathbf{U}}(\varepsilon) | q' \rangle \approx \int \frac{dp}{(2\pi\hbar)^n} \exp \left\{ \frac{i}{\hbar} [p(q - q') - \varepsilon H(q, p)] \right\}. \quad (73)$$

The approximate expression for the Hamiltonian path integral will be

$$\begin{aligned} \langle q | \hat{\mathbf{U}}_{t-t'} | q' \rangle &\approx \int \prod_{h=1}^{N-1} \frac{dp_h dq_h}{(2\pi\hbar)^n} \frac{dp_0}{(2\pi\hbar)^n} \\ &\times \exp \left\{ \frac{i}{\hbar} \sum_{h=1}^N [p_{h-1}(q_h - q_{h-1}) - \varepsilon H(q_h, p_{h-1})] \right\}, \end{aligned} \quad (74)$$

where  $q_N = q, q_0 = q'$ ; going to the limit  $N \rightarrow \infty$ , we obtain the standard representation for  $\mathbf{U}_{qq'}$  in the form of the path integral

$$\langle q | \hat{\mathbf{U}}_{t-t'} | q' \rangle = \int \prod_t \frac{dq(t) dp(t)}{(2\pi\hbar)^n} \exp \left\{ \frac{i}{\hbar} \int_{t'}^t [p\dot{q} - H(q, p)] dt \right\}. \quad (75)$$

We now make some comments about this well-known derivation.

First, in (71) we have substituted the resolution of the identity  $|p\rangle\langle p|$  in the ket. If we were to do this in the bra, instead of (72) we would obtain

$$\langle p | H(\hat{q}, \hat{p}) | q' \rangle = H(q', p) \langle p | q' \rangle. \quad (76)$$

When such expressions are used, it is generally assumed that the Hamiltonian has the simplest form  $H = p^2/2 + V(q)$ . In this case, the function  $H(q, p)$  in (75) is identical to the classical Hamilton function and it is easy to prove the equal validity of the two ways, since the difference  $\varepsilon[H(q, p) - H(q', p)] \approx \varepsilon V_{,i} \Delta^i$  makes a contribution of higher order than  $\varepsilon$ . Clearly, for more complicated Hamiltonians containing products of noncommuting operators (for example, the sum  $\hat{q}\hat{p} + \hat{p}\hat{q}$ ) Eqs. (72) and (76) will be invalid, since in them the classical functions  $H(q, p)$  and  $H(q', p)$  are obtained by replacing the operators  $\hat{q}$  and  $\hat{p}$  in  $H(\hat{q}, \hat{p})$  by the classical variables  $q, p$  or  $q', p$ , whereas the matrix element  $\langle q | \hat{q}\hat{p} + \hat{p}\hat{q} | q' \rangle$  is equal to  $\langle q | p \rangle \langle p | q' \rangle (q + q')$ . The validity of the substitution  $q' \rightarrow q$  is here not obvious. This question will be analyzed below. The presence in  $\hat{H}$  of even more complicated expressions with noncommuting operators can strongly influence the usual form of the path integral (see below).

Second, the expression (75) is unsuitable for curvilinear coordinates. Indeed, in accordance with (A.3) the amplitude  $\langle q | p \rangle$  acquires the factor  $g^{-1/4}$ , i.e., the kernel (73) is multiplied by  $(gg')^{-1/4}$ . Since the volume

element in (4) also changes,  $dq \rightarrow \sqrt{g} dq$ , we conclude that in curvilinear coordinates the Hamiltonian path integral has the form<sup>11</sup>

$$\begin{aligned} \langle q | \hat{\mathbf{U}}_{t-t'} | q' \rangle &= (gg')^{-1/4} \int \prod_t \frac{dq(t) dp(t)}{(2\pi\hbar)^n} \\ &\times \exp \left\{ \frac{i}{\hbar} \int_{t'}^t [p\dot{q} - H(q, p)] dt \right\}, \end{aligned} \quad (77)$$

where  $g$  and  $g'$  are taken at the values of the limit arguments, i.e., at  $q$  and  $q'$ .

Finally, in deriving (77) we have not considered the spectra of the operators  $\hat{q}$  and  $\hat{p}$  in curvilinear coordinates, whether they are self-adjoint, etc. But these questions are important for the correct understanding of the formal expressions (75) and (77); they will be discussed below.

We shall discuss in more detail the question of the terms with noncommuting operators in the Hamiltonian. In the class of systems specified by Lagrangians of the type (9), the Hamilton operator has the form (A.32) and, using (A.2), we can represent it in the form

$$\begin{aligned} \hat{H}^s &= \frac{1}{2} g^{ij}(\hat{q}) \hat{P}_i \hat{P}_j + f^j(\hat{q}) \hat{P}_j + \mathcal{T}^*(\hat{q}); \\ \mathcal{T}^* &= V + h, \quad \hat{P}_j = \frac{\hbar}{i} g^{-1/4} \partial_j g^{1/4}, \end{aligned} \quad (78)$$

where

$$f^j = \frac{\hbar}{2i} g^{jk}_{,k} - A^j; \quad h = -\frac{\hbar^2}{2} g^{1/4} \square g^{-1/4} + \frac{i\hbar}{2} A^j_{,j} + \frac{1}{2} A_j A^j, \quad (79)$$

where  $A^j = g^{ij} A_{,i}$ , and  $\square$  is defined by Eq. (A.5). In (78), the operators  $\hat{P}$  stand to the right of  $\hat{q}$ ; we shall call this order the *standard* order (which explains the superscript of  $\hat{H}$ ). We shall say that the reverse order ( $\hat{P}$  to the left of  $\hat{q}$ ) is the *antistandard* order and denote it by the superscript "a". Substitution of  $\hat{H}^s$  in (72) gives as the function  $H(q, p)$

$$H^s(q, p) = q^{ij}(q) p_i p_j / 2 + f^j(q) p_j + \mathcal{T}^*(q). \quad (80)$$

We take a different Hamiltonian  $\hat{H}'$ , which differs from  $\hat{H}^s$  by the order in which the operators follow one another, i.e.,

$$\hat{H}'^a = \hat{P}_i \hat{P}_j g^{ij}(\hat{q}) / 2 + \hat{P}_j f^j(\hat{q}) + \mathcal{T}^*(\hat{q}). \quad (81)$$

Obviously, it is now more advantageous to use Eq. (76), and we then obtain

$$H'^a(q', p) = q^{ij}(q') p_i p_j / 2 + f^j(q') p_j + \mathcal{T}^*(q'). \quad (82)$$

The functions  $H^s$  and  $H'^a$  differ by the terms

$$\begin{aligned} H^s - H'^a &= \frac{1}{2} p_i p_j \left( g^{ij}_{,k}(q) \Delta^k - \frac{1}{2} g^{ij}_{,kl}(q) \Delta^k \Delta^l + \dots \right) \\ &+ p_j (f^j_{,k}(q) \Delta^k + \dots) + \mathcal{T}^*_{,k} \Delta^k + \dots \end{aligned} \quad (83)$$

Do they need to be taken into account in the expression (74)? If the difference (83) could be ignored, this would mean that for Hamiltonian path integrals the order of the noncommuting operators in  $\hat{H}$  is immaterial and that the essentially different Hamiltonians  $\hat{H}^s$  and  $\hat{H}'^a$  lead to the same path integral (75). Of course, this is not so, and the difference (83) must make a contribution to the integral that we must take into account.

Thus, we must consider which extraterms must be retained. To establish this, we write down the most

general expression for the infinitesimal action in (73) with extraterms:

$$S(q, q', p) \approx p_i c^i(q, \Delta) - \varepsilon \left[ \frac{1}{2} p_i p_j \bar{g}^{ij}(q, \Delta) - p_j \bar{f}^j(q, \Delta) - \bar{\mathcal{T}}(q, \Delta) \right], \quad (84)$$

where

$$\left. \begin{aligned} \bar{g}^{ij}(q, \Delta) &= g^{ij}(q) + a_k^{ij}(q) \Delta^k + a_{kl}^{ij}(q) \Delta^k \Delta^l + \dots; \\ \bar{f}^j(q, \Delta) &= f^j(q) + b_k^j(q) \Delta^k + \dots; \\ c^i(q, \Delta) &= \Delta^i + c_{jk}^i(q) \Delta^j \Delta^k + c_{jkl}^i(q) \Delta^j \Delta^k \Delta^l + \dots; \\ \bar{\mathcal{T}}(q, \Delta) &= \mathcal{T}(q) + \dots \end{aligned} \right\} \quad (85)$$

Substituting (84) instead of the action in the square brackets in (73) and integrating over  $p$ , we obtain

$$U_{qq'}(\varepsilon) \approx (g g')^{-1/4} \frac{(\det \bar{g}^{ij})^{-1/2}}{(2\pi i \varepsilon \hbar)^{n/2}} \exp \left\{ \frac{i}{\hbar} \left[ \frac{\bar{g}_{ij}(c^i - \varepsilon \bar{f}^i)(c^j - \varepsilon \bar{f}^j)}{2\varepsilon} - \varepsilon \bar{\mathcal{T}} \right] \right\}; \quad (86)$$

here  $\bar{g}_{ij}(q, \Delta)$  is the inverse of the matrix  $\bar{g}^{ij}$ ; the factor  $(g g')^{-1/4}$  is included in accordance with Appendix 1. Therefore, the problem has been reduced to the problem of allowing for the extraterms in the Lagrangian formalism, and the results obtained in Sec. 1 can be used. Expanding  $(\det \bar{g}^{ij})^{-1/2}$  in powers of  $\Delta$ , we see that substitution of the kernel (86) in the integral

$$\psi_v(q) \approx \int dq' V \bar{g}^{ij} U_{qq'}(\varepsilon) \psi_0(q') \quad (87)$$

leads to an expression analogous to (21) with an action of the type (22) in which as vectors  $\alpha$  and  $A$  and tensors  $B, C, \dots$  we take

$$\left. \begin{aligned} \alpha_i &= -\frac{1}{2} g_{jk} a_i^{jk}; \quad \alpha_{ij} = -\frac{1}{2} \left[ \frac{1}{4} (a_i^{hk} a_j^{hl} + 2g_{hk} g_{ln} a_i^{hm} a_j^{nl}) - a_i^{hk} \right]; \\ A_j &= -f_j; \\ B_{ijk} &= \frac{1}{2} (g_{il} c_{jk}^l + g_{jl} c_{ik}^l - g_{lm} g_{jn} a_k^{mn}); \\ D_{ij} &= g_{il} a_j^{ih} f_h - g_{lh} b_j^i - f_h c_{ij}^h; \\ C_{ijkl} &= \frac{1}{2} [g_{lm} g_{jn} (a_k^{mn} a_l^{nl} - a_{kl}^{ln}) - 2g_{jn} a_i^{mn} c_{hl}^{ln} + 2g_{jn} c_{ihl}^{ln} + c_{ij}^{ln} c_{hl}^{ln}], \end{aligned} \right\} \quad (88)$$

and  $V$  is replaced by

$$\tilde{V} = \mathcal{T} - f_i f^i / 2. \quad (89)$$

The indices are raised, lowered, and contracted by means of the metric tensor  $g_{ij}$  (for example,  $a_i^k \equiv g_{kl} a_i^{kl}$ ). The terms of higher order, which are not written out explicitly in (85), lead to a negligibly small term in the action (of the type  $\Delta^3, \Delta^5/\varepsilon, \dots$ ). Therefore, in the prelimit expression (74) it is necessary to retain the following extraterms when making a change of variables, when reordering the operators in the Hamiltonian, or when changing the point of expansion:

$$p \Delta^2, p \Delta^3, \varepsilon p \Delta, \varepsilon p^2 \Delta, \varepsilon p^2 \Delta^2. \quad (90)$$

As in the Lagrangian formalism, we here need a technique for dealing with such nonstandard terms. In the light of the results of Sec. 1, this presents no problem. We show that the expression (84) is equivalent to a standard action with a Hamiltonian of standard form, i.e., that in (73) with the action (84) we can make the substitution

$$S = p_i c^i(q, \Delta) - \varepsilon H(q, p, \Delta) \rightarrow p_i \Delta^i - \varepsilon H^{\text{eff}}(q, p) \equiv S^{\text{eff}}. \quad (91)$$

As is shown in Sec. 1, the action (22) is equivalent in the sense of (18) to the standard effective action (17), in

which the coefficient of  $\Delta$  and the effective potential are given by Eqs. (32) [the presence in (86) and (87) of  $q'$ -dependent factors does not change the equivalence rules]. Since we are interested in the effective Hamiltonian, we turn to Eq. (33), and using it we see that the action (84) with the nonstandard terms is equivalent to the effective action  $S^{\text{eff}}$  (91) in which

$$H^{\text{eff}}(q, p) = g^{ij} p_i p_j / 2 + f_{\text{eff}}^j p_j + \mathcal{T}^{\text{eff}}, \quad (92)$$

where

$$\left. \begin{aligned} f_{\text{eff}}^j &= i\hbar(\alpha^j - \tilde{B}^j) - A^j \equiv -A_{\text{eff}}^j; \\ \mathcal{T}^{\text{eff}} &= \tilde{\mathcal{T}} + \hbar^2 [C_{ijk} g^{ij} g^{kl} - B_{ijk} B^{(ij)k} + (\alpha_i \alpha_j / 2 - \alpha_{ij}) g^{ij}] \\ &\quad - i\hbar D_{jj} + g^{ij} A_i^{\text{eff}} A_j^{\text{eff}} / 2. \end{aligned} \right\} \quad (93)$$

Further, bearing in mind that the term bilinear in  $A^{\text{eff}}$  makes a contribution to  $\tilde{V}$  and to the terms proportional to  $\hbar$  and  $\hbar^2$ , we obtain, using the explicit expressions (88) and (89) (the one-dimensional case was considered in Refs. 87 and 32),

$$\left. \begin{aligned} f_{\text{eff}}^j &= f^j + i\hbar(a_{ik}^{jk} - c_{kk}^j - 2g^{jn} c_{kn}^k); \\ \mathcal{T}^{\text{eff}} &= \mathcal{T} + i\hbar(b_k^j - 2f^j c_{hj}^k) + \hbar^2 [3c_{nhk}^{kn} - a_{hn}^{kn} + 2c_{lh}^{kn} a_n^{ln} + c_{hn}^{kn} a_l^{ln} - 2(c_{hk}^{kn} c_{nl}^{ln} + c_{nm}^{kn} c_{hm}^{ln} + c_{mn}^{kn} c_{lm}^{ln})]. \end{aligned} \right\} \quad (94)$$

If the exponential in (87) is multiplied by a  $q'$ -dependent factor  $\gamma(q')$  [for  $U_{qq'}$  (86), this is  $g'^{1/4}$ ], then it can be included in  $\psi_0$ ; then the Schrödinger equation with Hamiltonian obtained from (92) by the substitution  $p_j \rightarrow -i\hbar \partial_j$  will be satisfied by the functions  $\gamma(q)\psi(q)$  [for (86),  $\tilde{\psi} = g^{1/4}\psi$ ]. The factor  $g^{1/4}$  can readily be eliminated formally by going over in (92) from  $p_j$  to  $\tilde{p}_j = -i\hbar g^{-1/4} \partial_j g^{1/4}$ ; we then conclude that the function  $\psi$  satisfies the Schrödinger equation with the Hamiltonian

$$H^{\text{eff}} = g^{ij}(\hat{p}) \tilde{p}_i \tilde{p}_j / 2 + f_{\text{eff}}^j(\hat{p}) \tilde{p}_j + \mathcal{T}^{\text{eff}}. \quad (95)$$

In a Hamiltonian path integral, extraterms can also appear in front of the exponential, for example, in the form of the factor  $1 + \alpha_i \Delta^i + \alpha_{ij} \Delta^i \Delta^j$  or, which is equivalent [see (37)], in the exponential. After integration over the momenta, they can be taken into account in accordance with the rule (38), i.e., to the infinitesimal action we add the terms  $-i\hbar \alpha_i \Delta^i - \varepsilon \hbar^2 (\alpha_i \alpha_j / 2 - \alpha_{ij}) g^{ij}$ . In accordance with Eq. (33), this is equivalent to adding to the Hamilton function the terms  $i\hbar \alpha^i (p_i + f_i) + (i\hbar)^2 \alpha_i \alpha_j g^{ij} / 2 + \hbar^2 (\alpha_i \alpha_j / 2 - \alpha_{ij}) g^{ij}$ . Therefore, for Hamiltonian integrals we have the rule

$$1 + \alpha_i \Delta^i + \alpha_{ij} \Delta^i \Delta^j \approx \exp \left\{ \frac{-i\varepsilon}{\hbar} [i\hbar \alpha^j (f_j + p_j) - \hbar^2 \alpha_{ij} g^{ij}] \right\}. \quad (96)$$

The vanishing of the terms bilinear in  $\alpha_i$  indicates that the presence in the action of other terms linear in  $\Delta$  does not affect the result (96). Thus, to the list (90) we must add the extraterms

$$\Delta, \Delta^2 \quad (97)$$

in the argument of the exponential or in the pre-exponential factor. For generality, we note that in pre-exponential factors containing the momenta it is necessary to retain the terms

$$p^n \Delta^k, k = 1, 2, \dots, n + 2. \quad (98)$$

Equations (90), (92)–(96) solve the problem of listing the significant extraterms and constructing the effective Hamiltonian.



# **The ordering problem and nonuniqueness of the expression (75)**

Our calculations answer the question of how the non-commutativity of the canonical variables is manifested in the Hamiltonian path integral.<sup>3)</sup> It is clear from Eqs. (83), (85), and (93) that the noncommutativity of the operators  $\hat{q}$  and  $\hat{p}$  is reflected in the need to take into account the extraterms. The two Hamiltonians  $\hat{H}^s$  (78) and  $H^a$  (81), which are indistinguishable from the point of view of classical physics, give different pictures in the quantum description, and the difference between these Hamiltonians is reflected in the appearance of the non-standard terms (83), which (apart from the last) must be taken into account.

Of course, besides the standard or antistandard order of the operators one can consider intermediate cases. For example, as the term linear in the momenta we could take  $\alpha p f(\hat{q}) + \beta f(\hat{q}) \hat{p} \equiv \hat{T}_\alpha$ ,  $\alpha + \beta = 1$ , which leads after calculation of the matrix element  $\langle q | \hat{T}_\alpha | q' \rangle$  in (71) to the appearance in the "Hamiltonian" of the expression

$$p[\alpha f(q') + \beta f(q)] = p[f(q_\alpha) + O(\Delta^2)]; q_\alpha = q - \alpha \Delta; \quad (99)$$

this corresponds to the choice  $q_\alpha \in [q, q']$  as the reference point, i.e., as the argument of the functions of the coordinates in (73) [or the choice  $q_{\alpha k} \in [q_k, q_{k-1}]$  in the prelimit integral (74)].

From what we have said, it can be seen that it is not sufficient to write the path integral in the form (75). For Hamiltonians of the general form (78), it is necessary to specify the point of the interval of division at which the functions in the integrand in the prelimit expression (74) are taken. If the functions are taken at the point  $q_\alpha$ , then, as in the case of the Lagrangian formalism, it is sufficient to endow the integral [or the Hamiltonian in (75)] with the index  $\alpha$ ,  $0 \leq \alpha \leq 1$ . This eliminates the ambiguity in the usually employed expression (75).

We note that the equivalence rules (94) have been found for the case  $\alpha = 0$ . It is helpful to establish analogous rules for arbitrary  $\alpha \in [0, 1]$ . It can be shown that these rules are valid for any  $\alpha$ , as for the Lagrangian formulation.

It is obvious that the expressions found above make it possible to find the connection between integrals corresponding to different reference points, i.e., they enable us to go over from an integral endowed with index  $\alpha$  to an integral with index  $\beta$ . The transition formula follows

<sup>3)</sup> Here and in Ref. 30 (see also Refs. 39 and 52) various aspects of the ordering problem in a Hamiltonian path integral are discussed. The discussion in Ref. 30 considers the association of a classical function with an operator  $\hat{U} = \exp(-i\hat{H}t/\hbar)$ ; depending on the choice made for the order of  $q$  and  $p$  in  $\hat{U}$ , different classical functions are obtained (even for a one-dimensional harmonic oscillator). In the present subsection, we are concerned with the ordering of the operators in the Hamiltonian and the connection between the order of the operators in  $\hat{H}$  and the form of the path integral. The problem of allowing for the order of the operators in the Hamiltonian of field theories was also considered in Ref. 88.

readily from (84) and (85), in which it is necessary to set  $c(q, \Delta) = \Delta$ , and as  $\bar{g}^{ij}, \bar{f}^j$  to take  $g^{ij}$  and  $f^j$  at the points  $q_\alpha$  or  $q_\beta$ . Expanding the functions  $g^{ij}(q_\alpha)$  and  $f^j(q_\alpha)$  in powers of  $\alpha\Delta$ , we calculate the tensors  $a$  and  $b$  in accordance with the definitions (85):

$$a_{ij}^{ij} = -\alpha g_{,h}^{ij}(q); a_{kl}^{ij} = \frac{\alpha^2}{2} g_{,hl}^{ij}(q); b_{ih}^{ij} = -\alpha f_{,h}^{ij}(q); \quad (100)$$

the expansions of the tensors  $g^{ij}(q_\beta)$  and  $f^j(q_\beta)$  are obtained from here by the substitution  $\alpha \rightarrow \beta$ . Then, using the result (94), we find that the corresponding  $H^{\text{eff}}$  differ by the terms

$$\delta H = H_\alpha - H_\beta \approx -i\hbar(\alpha - \beta) g_{,h}^{jk}(q) p_j - i\hbar(\alpha - \beta) f_{,j}^{ij}(q) - (\alpha^2 - \beta^2) g_{,ij}^{ij}(q)/2. \quad (101)$$

Since we intend to go over from  $q_\alpha$  to  $q_\beta$ , it is desirable to have  $q_\beta$  here on the right-hand side as argument. Expanding the functions of  $q$  in the neighborhood of the point  $q_\beta$  and ignoring the unimportant terms, we obtain  $\delta H_\beta \approx -i\hbar(\alpha - \beta) g_{,h}^{jk}(q_\beta) p_j - i\hbar(\alpha - \beta) f_{,j}^{ij}(q_\beta) - \frac{\hbar^2}{2}(\alpha - \beta)^2 g_{,ij}^{ij}(q_\beta).$

(102)

In deriving (102), we used the equivalence rule  $\Delta^i p_j \rightarrow i\hbar \delta_j^i$ , which follows from the fact that the tensor  $b_{ij}^{ij}$  in (85) is manifested solely by the term  $i\hbar b_{ij}^{ij}$  in  $\mathcal{H}^{\text{eff}}$ ; it is even simpler to use the fact that the term  $\Delta^i p_j$  in the function  $H$  arises from the commutator  $[\hat{q}^i, \hat{p}_j] = i\hbar \delta_j^i$  in the operator  $\hat{H}$ . One way or another, we finally obtain the following rule for going over from one reference point to another:

$$\int \prod_i \frac{dp_i dq_i}{(2\pi\hbar)^n} \exp \left[ \frac{i}{\hbar} \int_t^t (p\dot{q} - H_\alpha) dt \right] = \int (\beta) \prod_i \frac{dp_i dq_i}{(2\pi\hbar)^n} \exp \left[ \frac{i}{\hbar} \int_t^t (p\dot{q} - H - \delta H) dt \right], \quad (103)$$

where  $\delta H = \delta H_\beta$  is given by (102). This relation is analogous to (43); in its derivation, we could use the circumstance that the rules (94) are true for any  $q_\alpha$ .

It is instructive to consider one further aspect of the noncommutativity of the operators in the Hamiltonian. Suppose the operators  $\hat{q}$  and  $\hat{p}$  are arranged at random<sup>31</sup> (see also Ref. 46), as in the Hamiltonian (A.32) written in the form

$$\hat{H} = \frac{1}{2} g^{-1/4}(\hat{q}) \hat{p}_i \tilde{g}^{ij}(\hat{q}) \hat{p}_j g^{-1/4}(\hat{q}), \quad \tilde{g}^{ij} = V g^{ij}; \quad (104)$$

for simplicity we have set  $A_i = V = 0$ . We denote  $g^{-1/4} = \bar{g}$ . Then the matrix element of  $\hat{H}$  in (71) can, using (A.3), be written as

$$\langle q | \hat{H} | q' \rangle = \frac{1}{2} \bar{g}(q) \langle q | \hat{p}_i | p'' \rangle \langle p'' | \tilde{g}^{ij}(\hat{q}) | q'' \rangle \langle q'' | \hat{p}_j | p' \rangle \langle p' | q' \rangle \bar{g}(q') \\ = \int \frac{dp'' dq'' dp'}{(2\pi\hbar)^{2n} (g\bar{g})^{1/4}} \exp \left\{ \frac{i}{\hbar} [p''(q - q'') + p'(q'' - q')] \right\} \\ \times H(q, q'', q', p', p''), \quad (105)$$

where

$$H(q, q'', q', p', p'') = \bar{g}(q) p_i \tilde{g}^{ij}(q'') p_j \bar{g}(q')/2, \quad (106)$$

i.e., for the kernel (71) itself we have

$$\langle q | \hat{U}(\varepsilon) | q' \rangle \approx (g\bar{g})^{-1/4} \int \frac{dp'' dq'' dp'}{(2\pi\hbar)^{2n}} \\ \times \exp \left\{ \frac{i}{\hbar} [p''(q - q'') + p'(q'' - q') - \varepsilon H] \right\}. \quad (107)$$

This is the form that the kernel of the evolution operator takes if  $\hat{q}$  and  $\hat{p}$  follow one another as in (104). The path integral is defined, as before, by the expression

(4), but now using the functions (107). Clearly, it differs from the simple expression obtained if in (107) we replace  $H$  by the corresponding classical function  $g^{ij}p_i p_j/2$ . The analog of the integral (74) will appear as if we had split the time interval into twice the number of subintervals, i.e., not into  $N$  but into  $2N$ , although the coefficient of  $H$  is, as before,  $\varepsilon = (t - t')/N$ . The function  $H$  itself in (107) contains coordinates and momenta corresponding to neighboring intervals.

Let us find what happens if in (107) we first integrate over  $p'$  and then over  $q''$ . We obtain

$$U_{qq'}(\varepsilon) \approx (gg')^{-1/4} \int \frac{dp'' dq''}{(2\pi\hbar)^n} \exp \left[ \frac{i}{\hbar} p'' (q - q'') \right] \times \delta^{(n)} \left( q'' - q' - \frac{\varepsilon}{2} \bar{g} p'' \bar{g}'(q'') \bar{g}' \right) \approx (gg')^{-1/4} \int \frac{dp''}{(2\pi\hbar)^n |J|} \times \exp \left\{ \frac{i}{\hbar} p'' \left[ q - q' - \frac{\varepsilon}{2} \bar{g} p'' \bar{g}'(q'') \bar{g}' \right] \right\}, \quad (108)$$

where  $J = \det \left| \delta_{ij} - (\varepsilon/2) \bar{g} p'' \bar{g}'^{ki}(q'') \bar{g}' \right|$  and  $q''$  makes the argument of the  $\delta$  function in the integrand of (108) vanish. Obviously,  $q'' = q' + O(\varepsilon)$ , and therefore  $J \approx 1 - (\varepsilon/2) \bar{g} p'' \bar{g}'^{ij}(q') \bar{g}'$  and (108) can be rewritten in the form

$$U_{qq'} \approx (gg')^{-1/4} \int \frac{dp}{(2\pi\hbar)^n} \exp \left\{ \frac{i}{\hbar} p (q - q') - \varepsilon \left( \frac{1}{2} \bar{g} p_i p_j \bar{g}'^{ij}(q') \bar{g}' - \frac{\hbar}{2} \frac{\bar{g} \bar{g}'}{2} p_i \bar{g}'^{ij}(q') \right) \right\}. \quad (109)$$

Since here the expression in the round brackets is the matrix element of the operator  $\hat{H}$  written in the form

$$\hat{H} = \frac{1}{2} \bar{g} \hat{p}_i \hat{p}_j \bar{g}'^{ij} \bar{g} - \frac{\hbar}{2i} \bar{g} \hat{p}_i \bar{g}'^{ij} \hat{p}_j \bar{g}, \quad (110)$$

Eq. (109) corresponds to such a partial ordering of the operators  $\hat{q}$  and  $\hat{p}$  in  $\hat{H}$ . If we were to integrate in (107) over  $p''$  and  $q''$ , we would obtain a result corresponding to ordering:

$$\hat{H} = \frac{1}{2} \bar{g} \hat{g}^{ij} \hat{p}_i \hat{p}_j \bar{g} + \frac{\hbar}{2i} \bar{g} \hat{g}'^{ij} \hat{p}_i \hat{p}_j \bar{g}. \quad (111)$$

These calculations characterize the connection between the order in which the operators follow one another in the Hamiltonian and the form of the path integral, which preserves the information about the mutual ordering of the operators.

#### On the formulation of Hamiltonian path integrals in curvilinear coordinates

In deriving Eqs. (73)–(76), we assumed tacitly that the spectra of the operators  $\hat{q}$  and  $\hat{p}$  extend from  $-\infty$  to  $+\infty$  and that the operators themselves are self-adjoint. But it can be seen from the following simple example that this is not the case. We consider the transition from Cartesian coordinates to cylindrical coordinates in three-dimensional space. The spectra of the operators  $x_i, p_i, i = 1, 2, 3$ , which occupy the entire real axis, are transformed into

$$\left. \begin{aligned} \hat{z} = \hat{x}_3 &: [-\infty, \infty]; \hat{p}_z = -i\hbar \partial_z &: [-\infty, \infty]; \\ \hat{r} = (\hat{x}_1^2 + \hat{x}_2^2)^{1/2} &: [0, \infty]; \hat{p}_r = -\frac{i\hbar}{\sqrt{r}} \partial_r \sqrt{r} &: [-\infty, \infty]; \\ \hat{\varphi} = \tan^{-1}(\hat{x}_2 \hat{x}_1^{-1}) &: [0, 2\pi]; \hat{p}_\varphi = -i\hbar \partial_\varphi &: 0, \pm\hbar, \pm 2\hbar, \dots \end{aligned} \right\} \quad (112)$$

Thus, even for this very simple transformation we encounter spectra of four types. The eigenfunctions of the operators  $\hat{p}_z, \hat{p}_r, \hat{p}_\varphi$  are

$$\frac{e}{\sqrt{r}} \exp \left[ \frac{i}{\hbar} (p_z z + p_r r + m\hbar \varphi) \right], \quad m = 0, \pm 1, \dots, \quad (113)$$

i.e., in expressions of the type (74) we shall encounter integrations with the most varied limits and also summation. In addition,  $\hat{p}_r$  is not a self-adjoint operator on the half-axis  $[0, \infty]$ ,<sup>57</sup> and its eigenfunctions are not orthogonal. All this influences the form of (74) and apparently makes it possible to use an expression of the form (77). At the same time, if the spectra of  $\hat{q}$  and  $\hat{p}$  fill the complete real axis in the curvilinear coordinates, then Eq. (77) is valid. Such a pronounced difference between systems of curvilinear coordinates appears somewhat unnatural. In reality, Eq. (77) is evidently valid irrespective of the form of the coordinates, i.e., it is possible to integrate with respect to all the variables in it, and, moreover, within infinite limits; true, in accordance with Sec. 1 the results of integration must be applied to functions suitably extended beyond the limits of the physical spectra, and the potential must also be redefined. At the present time, the proof of this assertion does not appear to be possible—it requires a general theory of the correspondence between canonical and unitary transformations. At the present time, such a theory does not exist,<sup>58,59</sup> and therefore we shall merely give some arguments in favor of what we have said.

The spectra (112) obviously exhaust the possible types of spectra of the operators  $\hat{q}$  and  $\hat{p}$  in the coordinate systems of greatest practical interest. We shall show that the summation over the discrete spectrum of  $\hat{p}_\varphi$  ( $m\hbar, m = 0, \pm 1, \dots$ ) can be replaced by integration over  $p_\varphi$  within infinite limits, a transition to infinite limits in the integral over  $\varphi$  being made simultaneously. The sum over  $m$  and the integral over  $\varphi$  in (87) can, using (73), be expressed as

$$\Psi_\varepsilon(\varphi) \approx \int_0^{2\pi} \frac{d\varphi'}{2\pi} \sum_{m=-\infty}^{\infty} \exp[i m (\varphi - \varphi')] f_\varepsilon(m\hbar) \Psi_0(\varphi'), \quad (114)$$

where  $f_\varepsilon(m\hbar)$  denotes an exponential with a matrix element of the Hamiltonian. We use the following device.<sup>14</sup> By means of the identities

$$\begin{aligned} \sum_{m=-\infty}^{\infty} F(m\hbar) &= \int_{-\infty}^{\infty} \frac{dp}{\hbar} F(p) \sum_{m=-\infty}^{\infty} \delta\left(\frac{p}{\hbar} - m\right); \\ \sum_{m=-\infty}^{\infty} \delta\left(\frac{p}{\hbar} - m\right) &= \sum_{m=-\infty}^{\infty} \exp(2\pi i p m / \hbar) \end{aligned} \quad (115)$$

we rewrite (114):

$$\Psi_\varepsilon(\varphi) \approx \sum_{m=-\infty}^{\infty} \int_0^{2\pi} \frac{d\varphi'}{2\pi} \int_{-\infty}^{\infty} dp_\varphi \exp \left[ \frac{i}{\hbar} p_\varphi (\varphi - \varphi' + 2\pi m) \right] f_\varepsilon(p_\varphi) \Psi_0(\varphi'). \quad (116)$$

Going over, as in Sec. 1, to the new function  $\Psi_0$ , which is defined in accordance with the condition  $\Psi_0(\varphi + 2\pi m) = \Psi_0(\varphi) = \psi_0(\varphi)$ ,  $\varphi \in [0, 2\pi]$  (or using the periodicity of  $\psi_0$ ), we find

$$\begin{aligned} &\sum_{m=-\infty}^{\infty} \int_0^{2\pi} \frac{d\varphi'}{2\pi} \exp(im\Delta_\varphi) f_\varepsilon(m\hbar) \Psi_0(\varphi') \\ &= \int_{-\infty}^{\infty} \int_0^{2\pi} \frac{dp_\varphi d\varphi'}{2\pi\hbar} \exp\left(\frac{i}{\hbar} p_\varphi \Delta_\varphi\right) f_\varepsilon(p_\varphi) \Psi_0(\varphi'), \end{aligned} \quad (117)$$

i.e., we now integrate over  $\varphi'$  and over  $p_\varphi$  within infinite limits. This device is fairly general.



If we integrate over the momentum variables within infinite limits, then for Hamiltonians of the type (78) the corresponding Gaussian integral can be calculated, and we arrive at a Lagrangian path integral. We can now go over to integration over infinite intervals, using the results found in Sec. 1. Obviously, the same result is obtained if from the very beginning (before integration over the momenta) we assume that all the variables range from  $-\infty$  to  $+\infty$ . Thus, it appears probable that we can integrate in (77) over all variables within infinite limits.

We now consider briefly the question of the non-self-adjointness of the operator  $p_r$  (112).<sup>57,60</sup> Its eigenfunctions  $\langle r|p\rangle = c \exp(i r p / \hbar) / \sqrt{r}$  are not orthogonal, and the integral

$$\langle p|p'\rangle = \langle p|r\rangle \langle r|p'\rangle = \frac{1}{2\pi\hbar} \int_0^\infty r dr \frac{1}{r} \exp\left[\frac{i}{\hbar}(p' - p)r\right] = \frac{i}{2\pi} \frac{1}{p' - p + i\varepsilon} \quad (118)$$

is not a  $\delta$  function (we ignore the variables  $z$  and  $\varphi$ ). However, on physical functions

$$\psi(p) = \langle p|r\rangle \langle r|\psi\rangle = (2\pi\hbar)^{-1/2} \int_0^\infty r dr \exp(-i p r / \hbar) \psi(r), \quad (119)$$

which are analytic for  $\text{Im } p < 0$  and decrease as  $\text{Im } p \rightarrow -\infty$ , the expression (118) is the kernel of the identity operator:

$$\langle p|p'\rangle \langle p'|\psi\rangle = \frac{i}{2\pi} \int_{-\infty}^\infty \frac{dp'' \psi(p'')}{p' - p'' + i\varepsilon} = \langle p|\psi\rangle. \quad (120)$$

There are two ways of going over to a Hamiltonian path integral in curvilinear coordinates. We have already considered one of them. In it, the Hamilton operator is written down in the new variables, and then the path integral is constructed; see above ("operator method"). The other method is associated with a change of variables in the prelimit expression (74). With regard to this second method, we note the following. As in the Lagrangian case (see Sec. 1), it is necessary to distinguish a change of variables in the integral and a canonical transformation. A change of variables is an operation that does not affect the end variables [for example,  $q$  and  $q'$  in (74)], to which the integration is not extended, and on the passage to the limit  $N \rightarrow \infty$  it is only necessary to ensure that all the important extraterms are kept. Although the new and old variables in the integrand may be related by a canonical transformation, such a change of variables does not entail a rotation of vectors in the Hilbert space (unitary transformation). The new variables may even be noncanonical. In other words, only the method of calculating  $U_{qq'}$  changes. In contrast, the change of variables corresponding to the operator method of transition to curvilinear coordinates must always be accompanied by a transformation of the "outermost" (nonintegrated) coordinates in the matrix element. It is such transformations that are of practical interest and are usually in mind. They correspond to a certain unitary transformation of all the state vectors and are considered below.

### 3. CANONICAL TRANSFORMATIONS AND HAMILTONIAN PATH INTEGRALS

#### Canonical and unitary transformations

To work with Hamiltonian path integrals, it is important to know their behavior under canonical transformations. This is a rather difficult question and relates to two problems: first, the general problem of the correspondence between canonical and unitary transformations<sup>41</sup>; second, the specific problem of the behavior of Hamiltonian path integrals under canonical transformations.

The importance of the first problem is obvious. Since the formalism of path integrals is a purely quantum formalism, it is clearly necessary to have a general theory of the behavior of probability amplitudes under such transformations. Dirac,<sup>3</sup> of course, made the well-known assertion that for systems having a classical analog the unitary transformations in quantum mechanics are analogous to canonical transformations. For infinitesimally small transformations, this analogy is almost obvious.<sup>3</sup> Overall, this problem is still far from its solution.<sup>58,59</sup> The nature of the difficulties encountered here is indicated by the following fact. Even with the simplest point transformation of the coordinates  $Q = q^2$  the ranges of variation of the new and the old variables are different, whereas unitary transformations obviously do not change the spectra of the operators (for further details on this point, see Ref. 58).

With regard to the second problem, the difficulties here are associated with the need to take into account the extraterms. As we have already noted, only the classical Hamilton function occurs in the path integrals in the description of the simplest systems; this creates the impression that the classical formulas suffice to study the question of canonical transformations. In fact, the situation is analogous to that in the Lagrangian formalism (see Sec. 1), in which it was necessary to retain in the path integrals extraterms that vanish in the classical limit. It is the same in the present case. For time-independent canonical transformations, the difference between the old and new infinitesimal actions is given by<sup>61</sup>

$$p\Delta q - P\Delta Q = \frac{\partial F_1(q, Q)}{\partial q} \Delta q + \frac{\partial F_1(q, Q)}{\partial Q} \Delta Q + O(\Delta^2), \quad (121)$$

where  $F_1(q, Q)$  is the generating function. If Eq. (121) is divided by  $\varepsilon$ , then, letting the time interval  $\varepsilon$  tend to zero, we obtain in the limit the well-known relation  $p\dot{q} - P\dot{Q} = dF_1/dt$ , since the terms of the type  $(\Delta q)^2/\varepsilon \approx \dot{q}\Delta q$  tend to zero together with  $\varepsilon$ . These terms cannot be ignored in the quantum description of the system, i.e., in the path integrals. As in Itô's formula (2), it is necessary to retain in (121) the terms  $O(\Delta^2)$ —and this is the key to the problem.

One further problem discussed below is associated with the construction of the operator of a unitary trans-

<sup>41</sup> Here and in what follows, the expressions *canonical transformation* and *unitary transformation* are applied to transformations in classical and quantum theories, respectively.

formation from a given generating function. It is obvious that this problem cannot be solved uniquely, and therefore in the present section we shall discuss canonical transformations defined by a generator. In addition, for simplicity we shall restrict ourselves below to a system with one degree of freedom (this is not a fundamental restriction). We first give explicit expressions for infinitesimal canonical and unitary transformations, which we shall use in what follows, and also the corresponding exact expressions for finite transformations. We consider the classical and quantum theories simultaneously.

### Infinitesimal transformation

We shall denote the original variables by the lower-case letters  $q^j, p_j, j=1, 2, \dots, n$ , and the transformed variables by upper-case  $Q^j, P_j$ . In addition, for brevity, we shall as a rule omit the indices, i.e., we shall write  $q, p, Q, P$ .

1. *Canonical transformation.* A canonical transformation can be specified by any one of four generating functions<sup>61</sup>:  $F_1(q, Q), F_2(q, P), F_3(p, Q), F_4(p, P)$ . For our purposes, it is most convenient to use the function  $F_2$ ; in this case, the transition from the old variables to the transition from the old variables to the new ones is made by means of the formulas

$$\partial F_2(q, P)/\partial q = p; \partial F_2(q, P)/\partial P = Q. \quad (122)$$

The infinitesimal canonical transformation is given by the function  $F_2^\omega = qP + G(q, P)\omega$ , where  $\omega$  is the parameter,  $\omega \rightarrow 0$ ; we shall call the function  $G$  the generator of the transformation. In accordance with (122),

$$p = P + \frac{\partial G(q, P)}{\partial q} \omega; \quad Q = q + \frac{\partial G(q, P)}{\partial P} \omega. \quad (123)$$

Since  $P = p + O(\omega)$ , we can, ignoring the terms of order  $\omega^2$ , write these formulas as

$$P = p - \frac{\partial G(q, p)}{\partial q} \omega; \quad Q = q + \frac{\partial G(q, p)}{\partial p} \omega. \quad (124)$$

After an infinitesimal time interval  $dt$ , the old and new actions differ by a total differential:

$$dt [p\dot{q} - H(q, p)] - dt [P\dot{Q} - \tilde{H}(Q, P)] = p dq - P dQ - dF_1(q, Q), \quad (125)$$

where  $p\dot{q} = p_j\dot{q}^j, p dq = p_j dq^j$ , etc., and  $\tilde{H}(Q, P) \equiv H[q(Q, P), p(Q, P)]$ . Knowing the function  $F_2$ , we can find  $F_1$  (and vice versa):

$$F_1(q, Q) = F_2(q, P) - QP; \quad (126)$$

here,  $P = P(q, Q)$  is a solution of the second equation of the system (122). For infinitesimal transformations,

$$F_1^\omega(q, Q) = P(q, Q) + G(q, P)\omega. \quad (127)$$

2. *Unitary transformation.* The unitary transformation corresponding to the canonical transformation (124) is given by the generator  $\hat{G}$ , which we define by the formula

$$\hat{G} = G(\hat{q}, \hat{p}), \quad (128)$$

i.e.,  $\hat{G}$  is obtained by the substitution  $q, p \rightarrow \hat{q}, \hat{p}$  in the function  $G(q, p)$ , and  $[\hat{q}, \hat{p}] = i\hbar$ . It is assumed that: a)

the substitution is made in Cartesian coordinates; b) some solution is found to the problem of the order in which the operators follow each other in  $\hat{G}$ , so that the operator  $\hat{G}$  is self-adjoint. The finite unitary transformation is realized by the operator

$$\hat{U}_\tau = \exp[-(i/\hbar)\hat{G}\tau] \quad (129)$$

( $\tau$  is the parameter of the transformation) in accordance with the rule

$$\hat{A}_\tau = \hat{U}_\tau^\dagger \hat{A} \hat{U}_\tau; \quad |\tau A'\rangle = \hat{U}_\tau^\dagger |A'\rangle, \quad (130)$$

where  $\hat{A}$  is an arbitrary operator, and  $|\tau A'\rangle$  is an eigenvector of the operator  $\hat{A}_\tau$  with eigenvalue  $A'$ . For infinitesimal transformations ( $\tau \equiv \omega \rightarrow 0$ ) we have

$$\left. \begin{aligned} \hat{q}_\omega &= \hat{q} + \frac{i}{\hbar} [\hat{G}, \hat{q}] \omega = \hat{q} + \frac{\partial \hat{G}(\hat{q}, \hat{p})}{\partial \hat{p}} \omega; \\ \hat{p}_\omega &= \hat{p} + \frac{i}{\hbar} [\hat{G}, \hat{p}] \omega = \hat{p} - \frac{\partial \hat{G}(\hat{q}, \hat{p})}{\partial \hat{q}} \omega. \end{aligned} \right\} \quad (131)$$

To bring out the analogy with Eqs. (124), we have here introduced the symbols of derivatives with respect to operators, the definition of which is obvious. Equations (131) define explicitly the infinitesimal unitary transformation of the variables  $\hat{q}$  and  $\hat{p}$  corresponding to the infinitesimal canonical transformation (124).

### Finite transformations

In the classical and quantum theories, they are given, respectively, by the generating function  $F_1(q, Q)$  [or  $F_2(q, P)$ ] and the operator  $\hat{U}_\tau$ . We shall show how to construct  $F_1(q, Q)$  and  $F_2(q, P)$ , given the function  $G(q, P)$ , and we shall find a representation for the kernel of the operator  $\hat{U}_\tau$  in the form of a path integral.

1. *Canonical transformation.* If  $\tau$  is the parameter of the finite transformation, Eqs. (124) can be rewritten in the form of the equations

$$\left. \begin{aligned} \dot{p}(\tau) &= -\partial G(q, p)/\partial q(\tau); \\ \dot{q}(\tau) &= \partial G(q, p)/\partial p(\tau), \end{aligned} \right\} \quad (132)$$

in which the derivatives  $df(\tau)/d\tau$  with respect to the parameter  $\tau$  are denoted by  $\dot{f}(\tau)$ . Let  $q(0) = q, p(0) = p, q(\bar{\tau}) = Q, p(\bar{\tau}) = P$  ( $\bar{\tau}$  is a finite value of the parameter  $\tau$ ); then the solutions of Eqs. (132) give in explicit form expressions for the new coordinates in terms of the old:  $Q = Q(q, p, \bar{\tau}), P = P(q, p, \bar{\tau})$ .

We shall find the function  $F_2$ . For this, we first find  $F_1$ . In accordance with (127),

$$F_1^\omega(q, Q) = [-P\dot{q} + G(q, P)]\omega \equiv -K(q, Q)\omega, \quad (133)$$

where  $\dot{q}\omega = Q - q, q = p(\tau), Q = q(\tau + \omega), P = p(\tau + \omega)$  and instead of  $P$  we have substituted the solution of the second equation (of the system of equations) in (132). It is easy to show that the solutions of the equations

$$\frac{d}{d\tau} \frac{\partial K(q, Q)}{\partial q} - \frac{\partial K(q, Q)}{\partial Q} = 0 \quad (134)$$

together with the condition  $\partial K/\partial Q = p$  give the same canonical transformation as the solutions of Eqs. (132) (cf. the proof of the equivalence of the Lagrangian and Hamiltonian equations in analytical mechanics—the

analogy here is complete). We shall show that the generating function  $F_1(q, Q)$  of a finite transformation is an extremum (minimum) of the functional  $-\int K(\dot{q}, q) d\tau$  [the boundary conditions for  $q(\tau)$  are fixed:  $q(0) = q, q(\bar{\tau}) = Q$ ]:

$$-F_1(q, Q) \equiv R(q, Q) = \text{extr} \int_0^{\bar{\tau}} K(\dot{q}, q) d\tau. \quad (135)$$

Obviously, the functional (135) takes extremal values on the solutions of Eqs. (134). It is also clear that the equations

$$\partial F_1(q, Q)/\partial q = p, \quad \partial F_1(q, Q)/\partial Q = -P \quad (136)$$

which follow from the definition (125), and Eqs. (132) or (134) define the same canonical transformation. Indeed, in accordance with (135), i.e., if Eqs. (134) are satisfied,  $\delta F_1 = -\partial K/\partial \dot{q} \delta q|_0^{\bar{\tau}}$ , and using the equations  $\partial K/\partial \dot{q} = p(\tau), p(0) = p, p(\bar{\tau}) = P$  we obtain  $\delta F_1 = -p \delta q(\bar{\tau}) + p \delta q(0)$ , i.e., Eqs. (136). This proves the equivalence of Eqs. (134) and (136). Therefore, (135) does indeed define the function  $F_1(q, Q)$  which occurs in (125). The function  $F_2(q, P)$  is related to  $F_1(q, Q)$  by (126), in which  $Q$  is replaced by the solution of the equation  $\partial F_1/\partial Q = -P$ . Equations (133) and (135) show how the generating function of the finite transformation is constructed from the given generator.

**2. Unitary transformation.** By means of the standard procedure (see Sec. 2), the matrix element  $\langle Q | \hat{\mathcal{U}}_{\bar{\tau}} | q \rangle$  can be represented by the Hamiltonian path integral

$$\langle Q | \hat{\mathcal{U}}_{\bar{\tau}} | q \rangle = \int_{q(0)=q}^{q(\bar{\tau})=Q} \prod_{\tau} \frac{dp d\dot{q}}{(2\pi\hbar)^n} \exp \left\{ \frac{i}{\hbar} \int_0^{\bar{\tau}} [p\dot{q} - G(q, p)] d\tau \right\}. \quad (137)$$

We emphasize that the expression (137) is well-defined only when we specify the order in which the operators follow one another in the generator  $\hat{G}$ , whose matrix element  $G(p, q)$  occurs here. Suppose the operators  $\hat{p}$  stand to the right of  $\hat{q}$ ; then  $G(q, p)$  is determined by the equation  $G(q, p) \langle q | p \rangle = \langle q | \hat{G} | p \rangle$ . We assume that the function  $G$  contains not more than second powers of the momenta. Then, integrating in (137) with respect to the momenta, we obtain

$$\langle Q | \hat{\mathcal{U}}_{\bar{\tau}} | q \rangle = \int \mathcal{D}q(\tau) \exp \left\{ \frac{i}{\hbar} \int_0^{\bar{\tau}} K(\dot{q}, q) d\tau \right\}. \quad (138)$$

This is an exact expression for the kernel of the unitary operator  $\hat{\mathcal{U}}_{\bar{\tau}}$ . Going to the limit  $\hbar \rightarrow 0$ , for functions  $K(\dot{q}, q)$  bilinear in  $\dot{q}$ , we obtain, using (135), the well-known quasiclassical approximation for this kernel<sup>7,8</sup>:

$$\langle Q | \hat{\mathcal{U}}_{\bar{\tau}} | q \rangle \approx \frac{D^{1/2}}{(2\pi i \hbar)^{n/2}} \exp \left[ \frac{i}{\hbar} R(q, Q) \right]; \quad D = \det \left| -\frac{\partial^2 R}{\partial q^i \partial Q^k} \right|. \quad (139)$$

In principle, the asymptotic behavior (139) can be obtained directly from (138) (see Ref. 62, p. 113, and also Ref. 41); however, it is simpler to use the Schrödinger equation  $i\hbar \partial \mathcal{U}/\partial \tau = G(Q, -i\hbar \partial/\partial Q) \mathcal{U}$  applied to the kernel  $\langle Q | \hat{\mathcal{U}}_{\bar{\tau}} | q \rangle$  written in the form (139). For the functions  $D$  and  $R$  we obtain equations analogous to Eqs. (A.23) and (A.25), by means of which we can readily show that the functions  $R$  and  $D$  in (135) and (139) do indeed satisfy these equations.<sup>7,8</sup>

**Example.** We consider an infinitesimal point transformation  $Q(q) = q + \varphi(q)\omega$ , where  $\varphi$  is an arbitrary

function. The transformation is given by the generator  $G(q, P) = P_i \varphi^i(q)$ , i.e., in accordance with (124)

$$P_j = p_j - \varphi_{,j}(q) p_i \omega; \quad Q^j = q^j + \varphi^j(q) \omega. \quad (140)$$

The corresponding quantum generator is

$$\hat{G} = \frac{1}{2} (\varphi^j(\hat{q}) \hat{p}_j + \hat{p}_j \varphi^j(\hat{q})) = \varphi(\hat{q}) \hat{p} + \frac{\hbar}{2i} \varphi_{,j}^j(\hat{q}). \quad (141)$$

Because  $G(q, P)$  is linear in the momenta, the ordering problem is solved by simple symmetrization, i.e., by the requirement that  $\hat{G}$  be Hermitian. For a unitary operator  $\hat{\mathcal{U}}_{\omega}$ , we have

$$\hat{\mathcal{U}}_{\omega} = \exp \left[ -(i/\hbar) \hat{G}(\omega) \right].$$

The wave functions transform in accordance with the formula

$$\begin{aligned} \tilde{\psi} &= \hat{\mathcal{U}}_{\omega}^{\dagger} \psi \approx \left( 1 + \omega \varphi^i \frac{\partial}{\partial q^i} + \frac{\omega}{2} \varphi_{,j}^j \right) \psi(q) \\ &\approx \left( 1 + \frac{\omega}{2} \varphi_{,j}^j(q) \right) \psi(q + \varphi(q)\omega) \approx J^{1/2} \psi(Q(q)), \end{aligned} \quad (142)$$

where  $J = \det Q_{,j}^i \approx 1 + \varphi_{,j}^j \omega$  is the Jacobian of the transformation. If the original coordinates are Euclidean, then  $J = \sqrt{g}$ , where  $g_{ij}$  is the new metric. It follows in particular from (142) that the operation of the change of variables  $\psi(q) \rightarrow \psi[Q(q)]$  is not unitary (the factor  $J^{1/2} = g^{1/4}$  must be added); it is "unitary" in the scalar product (under the integral sign), since  $dq \rightarrow J dq$ . It is easy to establish the law of transformation of the operators:

$$\langle q | \tilde{A} | q' \rangle = (J(q) J(q'))^{1/2} \langle Q(q) | A | Q(q') \rangle. \quad (143)$$

In Appendix 1, it is shown that in a nontrivial metric the kernels of the operators acquire the factor  $(gg')^{-1/4}$ , whereas (143) contains  $(gg')^{1/4}$ . The point is that, first, the use of kernels with the factor  $(gg)^{-1/4}$  presupposes integration with the invariant measure  $\tilde{d}q = \sqrt{g} dq$ , whereas here we understand integration with the measure  $dq$ ; second, the operators  $\tilde{A}$  act on the space of the functions  $\tilde{\psi}$ , whereas the kernel  $\langle q | \tilde{A} | q' \rangle / (gg')^{1/4}$  acts on the space of the functions  $\psi[Q(q)]$ .

## Canonical transformations of Hamiltonian path integrals

The results of Sec. 2 and those given above make it possible to attack the problem of the behavior of Hamiltonian path integrals under canonical transformations. To elucidate the problems that are encountered, we return to the simplest formula

$$\psi_{\epsilon}(q) \approx \int \frac{dq'' dp''}{2\pi\hbar} \exp \left\{ \frac{i}{\hbar} [p''(q - q'') - \epsilon H(q'', p'')] \right\} \psi_0(q''). \quad (144)$$

For simplicity, we consider a system with one degree of freedom ( $n=1$ ) and with the standard Hamiltonian [see (150)], and then discuss the generalization. The infinitesimal canonical transformation (124):  $q'' \rightarrow q', p'' \rightarrow p'$  (the role of  $Q, P$  are played by  $q'', p''$ —essentially, we are making the inverse transformation) obviously reduces to a simple change of variables in (144). Transforming similarly the variables  $q, p \rightarrow \tilde{q}, \tilde{p}$  and ignoring the terms of order  $\omega^2$ , we rewrite Eq. (144) as

$$\begin{aligned} \psi_{\epsilon} &\approx \int \frac{dq' dp'}{2\pi\hbar} \exp \left\{ \frac{i}{\hbar} p' \frac{\partial G(\tilde{q}, \tilde{p})}{\partial \tilde{p}} \omega + \frac{i}{\hbar} p' (\tilde{q} - q') - \epsilon H_{\omega}(q', p') \right\} \\ &\quad - \frac{i}{\hbar} p' \frac{\partial G(q', p')}{\partial p'} \omega - \frac{i}{\hbar} (\tilde{q} - q') \frac{\partial G(q', p')}{\partial q'} \omega \Big\} \psi_0 \left( q' + \frac{\partial G(q', p')}{\partial p'} \omega \right), \end{aligned} \quad (145)$$

where  $H_{\omega}(q', p') = H(q' + \omega \partial G/\partial p', p' - \omega \partial G/\partial q')$ . The



corresponding expression for the unitary transformation (129)–(131) is obtained as follows. By definition,

$$\psi_\varepsilon(q) = \langle q | \hat{U}_\varepsilon | \psi_0 \rangle = \langle q | \hat{U}_\omega \hat{U}_\varepsilon \hat{U}_\omega^\dagger | \psi_0 \rangle, \quad (146)$$

where  $\hat{U}_\varepsilon^\omega = \hat{U}_\varepsilon^\dagger \hat{U}_\omega = \exp(-i H_\omega \varepsilon / \hbar)$ . Using twice in (146) the resolution of the identity with respect to the complete system of eigenfunctions of the operator  $\hat{q}$ , and also the expressions for the matrix elements of the operators  $\hat{U}_\omega$ ,  $\hat{U}_\varepsilon^\omega$ , and  $\hat{U}_\varepsilon^\dagger$ , which are analogous to Eq. (73), we obtain

$$\psi_\varepsilon(q) \approx \int \frac{dP dQ}{2\pi\hbar} \frac{dP' dQ'}{2\pi\hbar} \frac{dp' dq'}{2\pi\hbar} \exp \left\{ \frac{i}{\hbar} [P(q-Q) - \omega G(q, P) + P'(Q-Q') - \varepsilon H_\omega^\alpha(Q', P') + p'(Q'-q') + \omega G(q', p')] \right\} \psi_0(q'). \quad (147)$$

This expression requires explanations. In accordance with (130) and (131),

$$\hat{H}_\omega = H(\hat{q}_\omega, \hat{p}_\omega) = H \left( \hat{q} + \frac{\partial G}{\partial p} \omega, \hat{p} - \frac{\partial G}{\partial q} \omega \right), \quad (148)$$

i.e., in  $\hat{H}_\omega$  the operators  $\hat{q}$  and  $\hat{p}$  are not ordered. To obtain Eq. (147), it is necessary to order the operators in the expression (148). We place  $\hat{p}$  to the left of  $\hat{q}$  (of course, bearing in mind that these operators do not commute). Then the matrix element of the operator that is then defined,

$$\langle P' | H_\omega^\alpha(\hat{q}, \hat{p}) | Q' \rangle = H_\omega^\alpha(Q', P') \langle P' | Q' \rangle, \quad (149)$$

gives the function written down in (147). For the standard method of ordering ( $\hat{p}$  to the right of  $\hat{q}$ ), we should have the function  $H_\omega^\alpha(Q, P')$  in Eq. (147); for our purposes, it is convenient to take the function  $H_\omega^\alpha$ . Obviously, in (147) it is necessary to take into account all terms of order  $\varepsilon, \omega, \varepsilon\omega$ . We make some comments concerning Eqs. (145) and (147).

It can be seen from Eq. (147) that the result of applying the unitary transformation appears to differ very strongly from the analogous result (145) obtained by canonical transformation of the variables in (144). It is clear from general considerations that Eqs. (145) and (147) define the same transformation, but it is desirable to have a direct proof of this.

As noted in Sec. 2, it is necessary to distinguish a change of variables in the prelimit integral and the transition to new variables (to a new representation) in quantum mechanics. In contrast to the second operation, the first does not entail a rotation of the vectors in the Hilbert space and is merely a device for calculating the multidimensional integral. The second operation is in practice more important, since, as a rule, a transition to new variables is dictated by the physics of the problem. It is this circumstance that to a large degree determines the importance of the problem of canonical transformations of Hamiltonian path integrals.

Although, as we shall see, the proof of the identity of Eqs. (145) and (147) is fairly long, it is also instructive. First, the calculations will illustrate Eq. (121) and make it clear why it is necessary to take into account in it the terms  $O(\Delta^2)$ . Second, we shall become acquainted with a case when it is necessary to take into account extraterms of even higher order ( $\Delta^4$ ) than the

terms (90) and (97). These features of the problem are obviously due to the presence of the two small parameters  $\varepsilon$  and  $\omega$  and the need to retain terms of order  $\varepsilon\omega$ .

We make the corresponding calculation. The most natural path to our goal is to integrate in (147) with respect to  $P, Q, P', Q'$ . This can be done explicitly only if the functions  $H$  and  $G$  contain the momenta to not higher than the second power. We restrict ourselves to functions of the form

$$H(q, p) = p^2/2 + V(q); \quad G(q, p) = \alpha p^2/2 + U(q) \quad (150)$$

( $\alpha$  is an arbitrary parameter). Then

$$H_\omega^\alpha(\hat{q}, \hat{p}) = H(\hat{q}, \hat{p}) - \hat{p}Y(\hat{q})\omega - \frac{i\hbar}{2}Y'(\hat{q})\omega + O(\omega^2), \quad (151)$$

where

$$Y(q) = U'(q) - \alpha V'(q); \quad Y' = dY/dq. \quad (152)$$

We note in passing that the function  $H_\omega(q', p')$  in Eq. (145) corresponds to only the first two terms in (151). Integration with respect to  $Q$  in (147) gives a  $\delta$  function in  $P - P'$ , which is removed by the final integration with respect to  $P$ . Omitting the primes of  $Q'$  and  $P'$  in the obtained integral, we have

$$\psi_\varepsilon(q) \approx \int \frac{dP dQ}{2\pi\hbar} \frac{dp' dq'}{2\pi\hbar} \exp \left\{ \frac{i}{\hbar} [-G(q, P)\omega + P(q-Q) - \varepsilon H_\omega^\alpha(Q, P) + p'(Q-q') + G(q', p')\omega] \right\} \psi_0(q'). \quad (153)$$

The next step is to integrate in (153) with respect to  $P$ . We write  $q - Q = \Delta_\omega$ . In the exponential in the integrand the coefficient of  $P^2$  is  $\varepsilon + \alpha\omega \equiv \Omega$ . This fact and also the necessity of retaining terms of order  $\varepsilon\omega$  means that the equivalence rules from Sec. 2 cannot be applied in a pure form, although the general method is valid here too. Integrating over  $P$ , we obtain

$$\psi_\varepsilon(q) \approx \int \frac{dQ dp' dq'}{2\pi\hbar (2\pi i \Omega \hbar)^{1/2}} \exp \left\{ \frac{i}{\hbar} \left[ \frac{[\Delta_\omega + \varepsilon\omega Y(Q)]^2}{2\Omega} - p'\Delta_\omega - U(q)\omega - V(Q)\varepsilon + \frac{i\hbar}{2}Y'(Q)\varepsilon\omega + p'(q-q') + G(q', p')\omega \right] \right\} \psi_0(q'). \quad (154)$$

The leading terms of the integral (154) as  $\varepsilon, \omega \rightarrow 0$  can be calculated by means of the standard procedure—expansion of the integrand in powers of  $\Delta_\omega$  and integration over  $Q$ , i.e., we again use Eq. (19), in which  $n=1, g_{ij} \rightarrow 1, g^{j_1 \dots j_{2k}} \rightarrow (2k-1)!!$  and  $\varepsilon \rightarrow \Omega$ . In the expansions of  $Y$  and  $V$  it is necessary to retain, respectively, the linear and quadratic terms, i.e.,  $Y(Q) \approx Y(q) - Y'(q)\Delta_\omega, V(Q) \approx V(q) - V'(q)\Delta_\omega + V''(q)\Delta_\omega^2/2$ , while in  $Y'(Q)$  the argument can be immediately replaced by  $q$ , since the coefficient of it is  $\varepsilon\omega$ . The difference from the equivalence rules in Sec. 1 is striking—we take into account the terms  $\varepsilon\Delta_\omega^2$ , which in accordance with (19) are equivalent to  $\varepsilon\Omega \approx \alpha\varepsilon\omega$ . For the same reason, in the expansion of  $\exp(p'\Delta_\omega/i\hbar)$  we must retain terms up to  $\Delta_\omega^4 \sim \Omega^2 \approx 2\alpha\varepsilon\omega$ . Of course, the terms  $\varepsilon\omega\Delta_\omega/\Omega$  must also be taken into account. Doing all this, we find

$$\psi_\varepsilon(q) \approx \int \frac{dp' dq'}{2\pi\hbar} \exp \left\{ \frac{i}{\hbar} \left[ -G(q, p')\omega + p'(q-q') - \varepsilon \left( \frac{p'^2}{2} + V(q) - U'(q)p'\omega + \frac{i\hbar\omega}{2}U''(q) \right) + G(q', p')\omega \right] \right\} \psi_0(q'). \quad (155)$$

It is now an easy matter to reduce the obtained expression to a form that can be compared with Eq. (145). The coefficient of  $p'^2/2$  in the exponential in (155) is  $\varepsilon$ , and therefore we can use the results of Sec. 2. We

make the following operations: (i) the substitution  $q \rightarrow q'$  in  $V(q)$  and  $U''(q)$ ; (ii) the substitution  $p'U'(q) \approx p'U'(q')\Delta$ ; (iii) the replacement of  $q$  by  $\tilde{q} + \omega \partial G(\tilde{q}, \tilde{p})/\partial \tilde{p}$ ; (iv) the shift of the variable of integration  $q' \rightarrow q' + \omega \partial G(q', p')/\partial p'$ . The validity of (i) is obvious—the old and new terms differ by quantities of the type  $\varepsilon \Delta$ . Using Eqs. (84), (92), and (94), in which all the tensors  $c$  and  $a$  are equal, and  $b_k^j \rightarrow -U''(q')$ , we make the substitution  $U''(q')p'\Delta \rightarrow i\hbar U''(q')$  in (155) after the operation (ii). Finally, bearing in mind that  $H(q' + \omega \partial G/\partial p', p' - \omega \partial G/\partial q') \approx H(q' + \omega \partial G/\partial p', p') - p'U'(q')\omega \equiv H_\omega(q', p')$ , we rewrite (155):

$$\Psi_\varepsilon(q) \approx \int \frac{dp' dq'}{2\pi\hbar} \exp \left\{ \frac{i}{\hbar} \left[ p' \frac{\partial G(\tilde{q}, \tilde{p})}{\partial \tilde{p}} \omega - G(\tilde{q}, p') \omega + p'(\tilde{q} - q') - \varepsilon H_\omega(q', p') + \frac{i\hbar}{2} U''(q') \varepsilon \omega - p' \frac{\partial G(q', p')}{\partial p'} \omega + G(q', p') \omega \right] \right\} \Psi_0 \left( q' + \frac{\partial G}{\partial p'} \omega \right). \quad (156)$$

This still differs from (145). We make the substitution

$$G(q', p') - G(\tilde{q}, p') \approx (q' - \tilde{q}) \frac{\partial G(q', p')}{\partial q'} - \frac{(q' - \tilde{q})^2}{2} \frac{\partial^2 G(q', p')}{\partial q'^2}. \quad (157)$$

We readily see, again using Eq. (19) or the rule (96), that in (157) we can make the substitution  $(\tilde{q} - q')^2 \rightarrow i\varepsilon\hbar$ . As a result, the terms of order  $\varepsilon\omega$  cancel and the obtained formula is identical to (145).

We now consider how we must make the infinitesimal canonical transformations in the Hamiltonian path integral. In accordance with our calculation, we can either 1) use the corresponding unitary operator to make the transformation  $\hat{H} \rightarrow \hat{H}_\omega$  and then the standard procedure to write down the path integral for the matrix element of the operator  $\hat{U}_t^\omega = \exp(-iH_\omega t/\hbar)$ , or 2) make an appropriate change of variables in the approximate expression for the Hamiltonian integral. This second possibility, which is natural when one is working with path integrals, is in practice more complicated for comparatively simple generators  $G$ . First, in accordance with Eq. (145) the obtained kernel acts on functions of the form  $\langle q + \omega \partial G/\partial p | \psi \rangle$ , whereas in accordance with (130) we are interested in the kernel of the operator in the space of the transformed functions  $\langle q | \omega \psi \rangle = \langle q | \mathcal{Q}_\omega^* | \psi \rangle$ . In other words, the kernel obtained by means of the canonical transformation must be modified accordingly (by applying the operators  $\mathcal{Q}_\omega^*$  and  $\mathcal{Q}_\omega$ ).

Second, one must take into account the extraterms scrupulously—which is a fairly tedious undertaking. Therefore, when making the canonical transformation it is more expedient to use the first approach. Then it is an easy matter to write down the transformed path integral:

$$\langle q | \hat{U}_t^\omega | q' \rangle = \int_{q(0)=q'}^{q(t)=q} \prod_t \frac{dp(t) dq(t)}{2\pi\hbar} \exp \left\{ \frac{i}{\hbar} \int_0^t [p\dot{q} - H_\omega(q, p)] dt \right\}, \quad (158)$$

where  $H_\omega$  is given by Eq. (149). The derivation of this expression by a change of variables in the approximate integral is described in Ref. 33.

We now turn to the question of finite canonical transformations. Suppose we are concerned with transformations that are specified by a generator and do not

change the ranges of the variables. Then obviously  $\hat{U}_t \rightarrow \hat{U}_t^\omega = \exp(-i\hat{H}_t^\omega/\hbar)$ , where

$$\hat{H}_t^\omega = \hat{U}_t^\dagger H(\hat{q}, \hat{p}) \hat{U}_t = H(\hat{q}_t, \hat{p}_t), \quad (159)$$

and the problem reduces to the standard procedure associated with Eqs. (4), (71), and (73). The corresponding expression will differ from (158) by  $\hat{H}_\omega^a \rightarrow \hat{H}_t^a$ . It should be recalled that the obtained path integral is to a large degree formal. Thus, even for generators  $G$  of the form (150) the operator  $\hat{H}_t$  can contain any powers of the momentum  $p$ , i.e., the integral over the momenta will not be Gaussian. In principle, such integrals can be given a rigorous meaning<sup>63, 64</sup> (one can define integrals of a more general form<sup>49</sup> without using an exponential), but they are of little use for calculations.

We note that the antistandard ordering [the superscript  $a$  in (158)] appeared for purely technical reasons in the proof of the identity of (145) and (147). Of course, we can go over in (158) to any other index following the rules of Sec. 2.

Let us discuss the expression (121) in somewhat more detail. The terms outside the square brackets in the exponential in (145) make the difference  $\delta = p''(q - q'') - p''(\tilde{q} - q')$ . In classical mechanics, this is a total differential  $dF_1$  if  $\Delta t = \varepsilon \rightarrow 0$  [see (125)]. As we have noted, for working with Hamiltonian path integrals such an approximation is insufficient. Bearing in mind that  $p'' = p' - \omega \partial G(q', p')/\partial q'$  and  $q - q'' = \tilde{q} - q' + O(\omega)$ , and ignoring terms of order  $\omega^2$ , we have

$$\delta \approx - \left[ p'(\tilde{q} - q) - p'(q' - q'') + (\tilde{q} - q') \frac{\partial G(q', p')}{\partial q'} \omega \right]. \quad (160)$$

Using now Eq. (157), and also the definition (127) of the function  $F_1^\omega(q', q'') = p'(q' - q'') + G(q', p')\omega$  (here, we must replace  $p'$  by the solution of the equation  $q'' = q' + \omega \partial G(q', p')/\partial p'$ ), we obtain

$$\delta = - \left[ F_1^\omega(\tilde{q}, q) - F_1^\omega(q', q'') - \frac{(\tilde{q} - q')^2}{2} \frac{\partial^2 G(q', p')}{\partial q'^2} \omega \right]. \quad (161)$$

It is obvious that in the classical case the ratio  $\delta/\varepsilon$  tends in the limit  $\varepsilon \rightarrow 0$  to  $-dF_1^\omega/dt$ , since the last term in the expression (161) gives zero in the limit. As we have seen, in Hamiltonian path integrals the last term cannot be ignored. It must be taken into account because of the presence of the "nonclassical" term  $i\hbar U''(q)\varepsilon\omega/2$  in Eq. (156), which appears because of the noncommutativity of the operators  $\hat{q}$  and  $\hat{p}$  [see (151)]. Thus, here, as before, the operator nature of the canonical variables is reflected in the extraterms.

Thus, the Hamiltonian path integral changes its form under canonical transformations, since, as we have seen, we cannot restrict ourselves to a replacement of the original classical Hamilton function by the transformed function because of the possible appearance in  $\hat{H}_\omega^a$  of the nonclassical terms  $-(i\hbar\omega/2)[U''(q) - \alpha V''(q)]$  [see (151)]. In this sense, the Hamiltonian path integral does not transform "covariantly" under canonical transformations. Strictly speaking, it is not covariant even under linear canonical transformations, when the func-



tion  $U(q)$  in (150) is quadratic in  $q$ , since even in this case the term  $Y'$ , which is proportional to  $\hbar$ , in (151) is nonzero ( $Y' = \text{const} \neq 0$ ). With regard to the  $S$  matrix, its transformation properties under the given transformations will not differ from the properties characteristic of arbitrary unitary transformations.

We have considered only generators of the form (150). To them, one can add terms linear in  $p$ ; as before, the calculations can be done. But if the function  $G$  contains higher powers of  $p$ , a corresponding analysis is impossible, since the integrals over the momenta cannot be calculated. Incidentally, this does not deprive the resulting formal expressions of meaning, since analogous expressions are also obtained for finite canonical transformations with generators in the class (150).

We now say a few words about arbitrary canonical transformations defined, not by a generator, but by a generating function  $F_1(q, Q)$ . In this case, it is probably impossible to construct an exact kernel of the corresponding unitary operator, since for this it is necessary to recover uniquely from  $F_1$  the generator  $G$  and then the corresponding operator  $\hat{G}$ . Although what we have said does not mean that such a canonical transformation does not correspond to some unitary transformation, the procedure described above for constructing the path integral in the new variables is unsuitable. In particular, a unique prescription for expressing the integral in the new variables is associated with the operator formalism, and this requires a quite definite order of noncommuting operators in the expressions of the old variables in terms of the new ones. The classical formalism, or rather the function  $F_1(q, Q)$ , does not contain such a prescription.

We consider finally point transformations in Hamiltonian path integrals. The transformation  $q, p \rightarrow Q, P, q^i = q^i(Q), P_i = d^i p_j, d^i_j = q^j_{,i}$  is linear in the momenta. The appearance of the extraterms is associated with the term  $p_i \Delta^i$  in the exponential, which is transformed into  $p_i c^i(Q, \Delta_Q)$ , where  $c^i$  is determined by Eqs. (85) and (60) (in the last, it is necessary to make the expansion at the point  $Q'$ ). We can now use the general equivalence rules (92)–(94) at the point  $Q'$ , taking the tensors  $a$  and  $b$  in them equal to zero, and making the substitutions

$$g_{ij} \rightarrow \tilde{g}_{ij} = d^k_i d^l_j g_{kl}, \quad f^i \rightarrow \tilde{f}^i = f^j (d^{-1})^i_j. \quad (162)$$

It must only be remembered that by virtue of the canonical invariance of the measure  $dq' dp$  the factor  $\sqrt{g'(g'g')^{-1/4}} = (g'/g)^{1/4}$  remains unchanged. To preserve the explicit covariance of the expression we must here too go over to the tensors  $\tilde{g}_{ij}$ , i.e.,  $(g'/g)^{1/4} = (\tilde{g}'/\tilde{g})^{1/4} (J/J')^{1/2}$ ,  $J = \det q^i_{,j}$ , and include the factor  $(J/J')^{1/2}$  by means of (96) in  $H_{\text{eff}}$ . By virtue of the invariance of the formalism,  $H_{\text{eff}}$  is obviously obtained from the old expression by the substitution (162) with allowance for the formulas analogous to (79) for  $H(q', p)$  [see (A.32)]. This proves the admissibility in the Hamiltonian integral of finite point transformations defined by a generating function.

## 4. HAMILTONIAN PATH INTEGRALS AND DYNAMICAL SYSTEMS WITH CONSTRAINTS

### Quantization of systems with constraints

The problem of quantizing the gravitational field stimulated the study of classical systems with constraints.<sup>65,66</sup> Dirac gave general rules for the quantum description of such systems.<sup>65</sup> Before we turn to path integrals, we state some results concerning their quantization that are important for what follows:

1) dynamical systems with constraints of the first and second class are quantized differently<sup>65</sup>;

2) for constraints of the first class, the operations of eliminating the unphysical variables and quantization do not commute.

We shall make some comments on the first proposition and prove the second. As is well known,<sup>67</sup> the constraints, i.e., functions  $\varphi_s(q, p), s = 1, 2, \dots, S$ , fixed by the condition  $\varphi_s = 0$ , can be regarded in the neighborhood of the physical region as part of the complete set of canonical variables. Since the existence of constraints of the second class means that it is necessary to fix simultaneously some of the canonically conjugate variables, i.e., variables of the type  $q^s$  and  $p_s$ , it follows automatically that the standard quantization procedure is inapplicable,<sup>65</sup> since the fixing of the variables brings one into conflict with the quantization condition  $[\hat{q}^s, \hat{p}_s] = i\hbar \delta^s_s$ . Therefore, in the presence of constraints of the second class the constraints must either be eliminated before quantization or (which is the same thing) one must go over from the Poisson brackets to the Dirac brackets<sup>65</sup> and then quantize using the new brackets. Since the Dirac brackets for constraints of the second class vanish, the canonical variables corresponding to these constraints remain classical after quantization (their commutator is equal to zero). In other words, in the case of quantization of a system with constraints of the second class using Dirac brackets it is immaterial at which stage the unphysical variables corresponding to these constraints are eliminated—before or after quantization.

Systems with constraints of the first class are quantized differently. In this case, the constraints  $\varphi_s$  play the part of canonical momenta conjugate to unphysical coordinates. They can also be fixed in the quantum description—the conditions  $\varphi_s = 0$  are transformed into conditions on the state vectors<sup>65</sup>:

$$\hat{\varphi}_s \psi_{\text{phys}} = 0. \quad (163)$$

Since in both cases, i.e., in the presence of constraints of both the first and second class, the matter reduces to a restriction of the original phase space to a certain subspace, which is determined solely by the physical variables, the following question arises: Does the difference in the quantization prescriptions affect the physics? Would it not be possible in the case of constraints of the first class too to eliminate first all the unphysical variables and then quantize? These questions are answered by the second of the propositions above. If we first eliminate the unphysical vari-



ables, and then go over to the quantum description, the physical picture will differ from the picture that arises in the case of the Dirac quantization (163). A difference arises in the physically most interesting systems when the eliminated variables are associated with curvilinear coordinates (in the case of elimination of variables associated with Cartesian coordinates, the two methods lead to the same result). The reason for the difference is simple—if the eliminated variables are associated with curvilinear coordinates, the standard quantization prescription (the substitution  $q, p \rightarrow \hat{q}, \hat{p}$ ,  $H(q, p) \rightarrow H(\hat{q}, \hat{p})$ ,  $[\hat{q}, \hat{p}] = i\hbar$ ) does not work for them; at the same time, the remaining physical variables need not retain information about their “curvilinear” origin. We demonstrate this by an example which simultaneously serves as the proof of proposition 2.<sup>31,32</sup> To prove it, it is sufficient to find one example of the asserted noncommutativity.

*Example.*<sup>51</sup> We consider the dynamical system defined by the Lagrangian

$$L(x, \dot{x}, y, \dot{y}) = [(d/dt - yT)x]^2/2 - V(x^2), \quad (164)$$

where  $x$  is a two-dimensional vector,  $x = (x_1, x_2)$ , and  $T = -i\tau_2$ , where  $\tau_2$  is a Pauli matrix;  $(Tx)_i = T_{ij}x_j$ . The theory is invariant under the gauge transformations

$$\delta y = \dot{\omega}(t); \quad \delta x = \omega(t)Tx, \quad (165)$$

where  $\omega(t)$  is an infinitesimally small arbitrary function of the time. Essentially, (164) is the Lagrangian of scalar electrodynamics in a (1+0) space, in which the electromagnetic field is  $A_\mu \rightarrow A_0 = y$ , and the complex “field”  $\varphi$  is expressed in the form  $\varphi = (x_1 + ix_2)/\sqrt{2}$ . Formally, this Lagrangian, which describes the motion of a particle of unit mass in the  $x$  plane, is the simplest example of a gauge theory.

A primary constraint is given by the equation  $\pi = \partial L / \partial \dot{y} = 0$ . The Hamiltonian is

$$H = p^2/2 + V(x^2) + ypTx, \quad (166)$$

and there is the secondary constraint  $\Phi = pTx = p_i T_{ij} x_j$ , since  $\{y, \pi\} = 1$ .

In accordance with Dirac's prescription,<sup>65</sup> we impose the following conditions on the physical state vectors on quantization:

$$\hat{\pi}\psi_{\text{phys}} = \hat{\Phi}\psi_{\text{phys}} = 0. \quad (167)$$

We shall find the equation that the physical wave vectors satisfy. Going over in (166) to operators,  $x \rightarrow \hat{x}$ ,  $p \rightarrow \hat{p}$ , we write the Hamiltonian in polar coordinates  $[(x_1, x_2) \rightarrow (r, \varphi)]$ :

$$\hat{H} = -\frac{\hbar^2}{2} \left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \varphi^2} \right) + V(r^2) + y\hat{p}_\varphi, \quad (168)$$

where  $p_\varphi = -i\hbar \partial / \partial \varphi = \hat{p}T\hat{x} \equiv \hat{\Phi}$ . Using (167), we conclude that the physical wave functions satisfy the equation

$$i\hbar \frac{\partial \psi_{\text{phys}}}{\partial t} = \left[ -\frac{\hbar^2}{2} \left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} \right) + V(r^2) \right] \psi_{\text{phys}}. \quad (169)$$

<sup>51</sup> The same example was in fact considered in Ref. 68. Models of this type with a non-Abelian gauge group were studied in Ref. 69.

This is the result given by Dirac's prescription (163). Let us consider what we obtain if we first eliminate the unphysical variables and then quantize. The classical Hamiltonian (166) in polar coordinates takes the form

$$H = (p_r^2 + p_\varphi^2/r^2)/2 + V(r^2) + yp_\varphi. \quad (170)$$

Eliminating the unphysical variables, i.e., setting  $p_\varphi = \varphi = 0$ , we obtain

$$H' = p_r^2/2 + V(r^2). \quad (171)$$

We have arrived at a one-dimensional problem on a half-axis. The quantization is done in the standard manner, and the operator

$$\hat{H}' = -\frac{\hbar^2}{2} \frac{\partial^2}{\partial r^2} + V(r^2) \quad (172)$$

is extended to a self-adjoint operator.<sup>57</sup> It is clear that the Hamiltonian in the Schrödinger equation (169) is not identical to the Hamiltonian (172). This proves proposition 2.

The considered example demonstrates one further feature of quantization with the condition (163), namely, after the transition to the physical phase subspace, information about the eliminated unphysical subspace is preserved. The physical vectors satisfying Eq. (169) form a subspace of the Hilbert space spanned by the eigenvectors of the operator (168). These last are normalized in accordance with the condition

$$\int_0^\infty r dr \int_0^{2\pi} d\varphi |\psi(r, \varphi)|^2 = 1. \quad (173)$$

The vectors  $\psi_{\text{phys}}$  satisfying the condition  $\hat{p}_\varphi \psi_{\text{phys}} = 0$  do not depend on  $\varphi$ , and for them (173) can be written in the form

$$2\pi \int_0^\infty r dr |\psi_{\text{phys}}(r)|^2 = 1, \quad (174)$$

i.e., the solutions of the one-dimensional equation (169) must be normalized in accordance with (174) (with weight that depends on the dimension of the unphysical configuration subspace; see also Refs. 68 and 70).

One further problem which arises on quantization of systems with constraints of the first class relates to the problem of ordering the operators in the constraints.<sup>71,72</sup> For Lagrangians of the considered class [functions bilinear in the velocities of the type (9)], the following procedure can be proposed. It is easy to show that for such systems the primary constraints  $\varphi_s^{(1)}$  are linear in the momenta,<sup>61</sup> and the problem of ordering in such operators can be uniquely (up to unitary equivalence) solved by requiring their Hermiticity<sup>3</sup> or by simple symmetrization (we assume that  $\varphi_s^{(1)}$  can be taken to be new canonical momenta). Suppose that the problem of ordering the operators in the Hamiltonian has also been solved. Then because of the absence of constraints of the second class all secondary constraints

<sup>61</sup> In the given case, the equations  $p_i + \partial L / \partial \dot{q}^i$  are linear in  $\dot{q}$  and  $p$ . If the rank of the matrix  $\partial^2 L / \partial \dot{q}^i \partial \dot{q}^j$  is  $R$ , then the solutions  $\dot{q}^i = f^i(q, p)R$  of the equations are also linear in the momenta. Substituting these solutions in the remaining equations, which gives the primary constraints, we see that the latter are linear in the momenta.

are obtained as follows. From (163) and the condition that the Hamiltonian does not carry  $\psi_{\text{phys}}$  out of the physical subspace, we obtain the conditions

$$(\hat{\psi}_s^{(1)}, \hat{H}) \psi_{\text{phys}} = \hat{\psi}_s^{(2)} \psi_{\text{phys}} = 0. \quad (175)$$

If these equations are satisfied automatically on vectors  $\psi_{\text{phys}}$  satisfying (163), then secondary constraints are absent. If not, we must restrict the Hilbert space further by requiring also fulfillment of the conditions (175). Obviously, the procedure must be continued, i.e., the commutator  $[\hat{\psi}^{(2)}, \hat{H}]$  must also vanish on the physical functions (we recall that all constraints are in involution, i.e.,  $[\hat{\psi}_s, \hat{\psi}_s] \psi_{\text{phys}} = 0$ ). This procedure makes it possible to find the constraints with allowance for the order of the operators in them.

We note that logically there are two methods of quantization in the presence of constraints of the first class: 1) one can first eliminate from the Hamiltonian all the unphysical variables and then quantize; 2) one can quantize using the condition (163). *A priori*, there do not appear to be reasons for giving preference to either of these ways. Only experience can decide this question. It is well known that quantum electrodynamics is constructed on the basis of a condition of the type (163).

#### Elimination of unphysical variables in a Hamiltonian path integral

Our analysis in conjunction with the results of Sec. 2 enables us to formulate rules for eliminating redundant degrees of freedom in the method of path integrals.

##### Constraints of the first class

The prescription here given by Faddeev<sup>73</sup> (modified subsequently in the monographs of Refs. 74–76) essentially corresponds to quantization after elimination of all unphysical variables (see Refs. 31 and 32 and Appendix 4.2). According to the example we have considered, it leads to results that differ from those which follow from the requirement (163). As we have noted, the two approaches lead to the same results only in the simplest cases when the unphysical variables are associated with Cartesian coordinates.

Thus, suppose we have a Hamiltonian  $\hat{H}$  and operators  $\hat{\psi}_s$  corresponding to constraints. Suppose that by means of a unitary transformation we can go over to new canonical variables  $\hat{q}, \hat{p} - \hat{Q}, \hat{P}; \hat{\chi}, \hat{\pi}, [\hat{Q}^r, \hat{P}_r] = i\hbar\delta_r^r$ ;  $[\hat{\chi}^s, \hat{\pi}_s] = i\hbar\delta_s^s$ ;  $[\hat{\chi}, \hat{Q}] = [\hat{\chi}, \hat{P}] = [\hat{\pi}, \hat{Q}] = [\hat{\pi}, \hat{P}] = 0$  such that some of the new momenta can be identified with the constraints:  $\hat{\pi}_s = \hat{\psi}_s(\hat{q}, \hat{p})$  (in the neighborhood of the physical region). We place the momenta  $\hat{\pi}$  (the constraints) in  $H(\hat{Q}, \hat{P}, \hat{\chi}, \hat{\pi})$  to the right of the operators of the coordinates (bearing in mind that they do not commute). Since the terms corresponding to the constraints give zero when the Hamiltonian is applied to a physical state, we can set these terms equal to zero. It is obvious that the remaining part  $\hat{H}|_{\hat{\pi}=0} = \bar{H}$  must not depend on  $\hat{\chi}$  [otherwise, by virtue of (175), it would contain certain  $\pi$ , which contradicts the assumption  $\hat{\pi} \rightarrow 0$ ], i.e., the condition  $[\hat{\pi}_s, \bar{H}] = 0$  must be satisfied. The operator  $\bar{H} = \hat{H}_{\text{phys}}$  is the required physical Hamil-

tonian. After elimination of the unphysical degrees of freedom, we can write down a path integral for the evolution operator using the general rules of Sec. 2. It can also be written down for an operator  $\hat{H}(\hat{Q}, \hat{P}, \hat{\chi}, \hat{\pi})$  that depends on  $\hat{\chi}$  and  $\hat{\pi}$ . Since the evolution operator is applied only to the physical states, which satisfy the conditions  $\hat{\pi}_{\text{phys}} = 0$ , i.e., do not depend on  $\chi$ , it is clear that the unphysical variables can be eliminated by introducing in the integrand the factor  $\Pi_s(2\pi\hbar)\delta(\chi^s)\delta(\pi_s)$ . This general procedure is inconvenient for practical use, since, as a rule, it is difficult to find  $\hat{H}$  in the new variables. It is desirable to have expressions with the Hamiltonian and constraints depending on the original variables  $q$  and  $p$ . For this, it is necessary to make a canonical transformation to the old variables in the obtained expression. The result will be the required formula. Unfortunately, the question of arbitrary canonical transformations in a Hamiltonian path integral remains open, and therefore we shall restrict ourselves below to the case, of practical importance, of constraints which can be obtained from the old variables by a point transformation. One can show that such constraints are linear in the momenta, so that the ordering problem, if it arises, can be solved by simple symmetrization.

Thus, in the new variables the formula for the physical  $\psi_{\text{eff}}$  with eliminated variables can be written in the form

$$\psi_{\text{eff}} \approx \int \frac{dQ' dP d\chi' d\pi}{(2\pi\hbar)^{n-s}} \left( \frac{g'}{g} \right)^{1/4} \prod_{s=1}^s \delta(\chi'^s) \delta(\pi_s) \exp \left\{ \frac{i}{\hbar} [P\Delta Q + \pi\Delta\chi - \varepsilon (\bar{H}_{\text{eff}}(Q', P) + H_1(Q', P, \chi', \pi))] \right\} \psi_0(Q'). \quad (176)$$

As in Sec. 3, the combination  $(g'/g)^{1/4}$  of determinants is associated with the fact that application of a kernel having the factor  $(gg')^{-1/4}$  presupposes integration with the measure  $\sqrt{g'}dq'$ . The subscript "eff" of  $\bar{H}$  means that this function is written down with allowance for the rules of commutation of the operators. Further,  $\Delta\chi = \chi - \chi'$ , so that in (176) we should set  $\chi = 0$ , but, bearing in mind the subsequent transition to the path integral, this has not been done. We can now return to the original variables, making the substitution  $Q = Q(q)$ ,  $P = P(q, p)$ ,  $\chi = \chi(q)$ ,  $\pi = \varphi(q, p)$  (point transformation); as  $\varphi_s(q, p)$ , we take the functions that occur in the equation

$$\langle p | \hat{\psi}_s(\hat{q}, \hat{p}) | q \rangle = \varphi_s(q, p) \langle p | q \rangle. \quad (177)$$

If (176) did not contain  $\delta$  functions, then with allowance for the extraterms we would obtain an integral in the original variables with the original Hamiltonian. The presence of the  $\delta$  functions makes it unnecessary to take into account the extraterms associated with the unphysical variables  $q^s$ , which are fixed by the additional conditions  $\chi^s = 0$ . As a result, we obtain, not the original Hamiltonian  $H(q, p)$ , but some effective Hamiltonian, and Eq. (176) can be rewritten as

$$\psi_{\text{eff}} \approx \int \frac{dq' dp}{(2\pi\hbar)^{n-s}} \prod_{s=1}^s \delta(\chi^s(q')) \delta(\varphi_s(q', p)) \exp \left\{ \frac{i}{\hbar} [p\Delta q - \varepsilon H_{\text{eff}}(q', p)] \right\} \psi_0(q'). \quad (178)$$

The explicit form of  $H_{\text{eff}}$  is determined by going over from (176) to (178); the factor  $(g'/g)^{-1/4}$  is included in the definition of  $H_{\text{eff}}$  (this can always be done, since  $g'/$



$g$  has the form  $1 + c\Delta + \dots$ ; see Secs. 1 and 2). The change in the Hamiltonian reflects the operator nature of the canonical variables. It is also associated with a feature of a change of variables in the presence of  $\delta$  functions—they annihilate not only the variables themselves but also the extraterms generated by them. From Eq. (178) we obtain the following representation for the kernel of the evolution operator:

$$\langle q | \hat{U}_t | q' \rangle = \int_{q(0)=q'}^{q(t)=q} (1) \prod_t \left[ \frac{dq dp}{(2\pi\hbar)^{n-s}} \right. \\ \left. \times \prod_{s=1}^S \delta(\chi^s(q)) \delta(\varphi_s(q, p)) \right] \exp \left[ \frac{i}{\hbar} \int_0^t (p\dot{q} - H_{\text{eff}}) dt \right]. \quad (179)$$

It should be borne in mind that the use of the kernel (179) presupposes integration with respect to the measure  $dq'$ , i.e., without the factor  $\sqrt{g'}$ . The main difference between this formula and (A.50) is associated with allowance, first, for the noncommutativity of the operation of elimination of the unphysical variables and the quantization operation; second, the noncommutativity of the operators not only in the Hamiltonian but also in the constraints; third, the specific properties of curvilinear coordinates [the appearance of the factor  $(gg')^{-1/4}$  in the kernels; see Sec. 2]; and fourth, the fact that the transition  $q, p \rightarrow Q, P, \chi, \varphi$  is a point transformation. At the present time, it is not possible to provide a justification of the formula for an arbitrary canonical transformation  $q, p \rightarrow Q, P, \chi, \varphi$  [and, *a fortiori*, a noncanonical transformation as in (A.50)]. The well-known difficulties also arise when allowance is made for the order of the operators in more complicated constraints, although they do not appear to be insuperable.

#### Constraints of the second class

Systems with constraints of the second class are encountered in quantum physics much less often. As an example, one can take a gauge vector field if its Lagrangian contains a mass term.<sup>77</sup> Thus, let  $\theta_1, \dots, \theta_{2s}$  be constraints of the second class, i.e.,  $\det\{\theta_\sigma \theta_\rho\} \neq 0$ . As we explained above, constraints of the second class must be eliminated before quantization (or retained as classical parameters after quantization), and it would therefore appear that in the integrand in (179) we could substitute  $\Pi_{t\sigma} \delta(\theta_\sigma) [\det\{\theta_\sigma \theta_\rho\}]^{1/2}$ .<sup>77</sup> This is in fact so if the physical configuration space is Euclidean and the physical coordinates Cartesian. Otherwise, the quantization procedure and the form of the integral are different (see Secs. 1, 2, and 5). It must be borne in mind that the transition from the Poisson brackets to the Dirac brackets<sup>65</sup> results in a change in the criterion of "canonicity," i.e., variables that are canonical from the point of view of the Poisson brackets need not be so from the point of view of the Dirac brackets. Formally, the unphysical variables are then also "quantized," the operators corresponding to them commuting with all the other operators. Therefore, in the presence of constraints of the second class it is first necessary to elucidate the nature of the physical subspace and the properties of the metric tensor  $g_{ij}^{\text{phys}}$ . If  $g_{ij}^{\text{phys}} \neq \text{const}$ , there is an ordering problem in the Hamiltonian and it is necessary to take into account the factor  $(g^{\text{phys}} g'^{\text{phys}})^{-1/4}$ . If, moreover, the configuration sub-

space has curvature, we must add to  $H$  the term  $\hbar^2 R/12$  (see Sec. 1). Finally, using a resolution of the identity with respect to a complete system of functions (see Sec. 2), we must take into account the features of the unphysical variables that we have noted. When using the analog of Eq. (179),

$$\langle q | \hat{U}_t | q' \rangle = \int_{q(0)=q'}^{q(t)=q} (1) \prod_t \frac{dq dp}{(2\pi\hbar)^{n-s}} \\ \times \prod_{\sigma}^{2S} \delta(\theta_\sigma) [\det\{\theta_\sigma, \theta_\rho\}]^{1/2} \exp \left[ \frac{i}{\hbar} \int_0^t (p\dot{q} - H_{\text{eff}}) dt \right], \quad (180)$$

it is necessary to reckon with all these circumstances.

The rules we have given do not pretend to universality. Thus, the physical phase space may be curved (in some gauge theories, the phase space is a cone<sup>69</sup>). In this case, the quantization rules are changed.<sup>78</sup> Moreover, the physical phase space may have a nontrivial topological structure, which complicated the problem still further. None of these possibilities are considered here. In the problem of eliminating unphysical variables in Hamiltonian path integrals several difficulties are encountered simultaneously. Besides the two mentioned at the beginning of Sec. 3, there is the inadequate development of the general (classical) theory of systems with constraints. We may here add the problem of formulating path integrals for systems with nontrivial (geometrical or topological) phase spaces. All this means that universal formulas for eliminating unphysical degrees of freedom are not to be expected in the too near future.

## CONCLUDING REMARKS

### On the Dirac-Feynman-Pauli-DeWitt quantization procedure

The assertion that the kernel of the operator of an infinitesimal shift in time is given by Eq. (12) is, in fact, an independent quantization postulate. Essentially, quantization means that one is given a classical Hamilton function (or Lagrange function, i.e., one knows the classical equations of motion) and specifies a law of variation of wave functions in time. The standard quantization procedure<sup>3</sup> reduces to the assertion that the wave functions of the system satisfy a Schrödinger equation in which the Hamilton operator is obtained from the Hamilton function by the replacement of the canonical variables by operators. The limitations of this prescription are due to the fact that, first, it is valid only in a Cartesian coordinate system and, second, it gives a result only when there is no ordering problem for the operators.<sup>3</sup> At the same time, the function (12) together with the action (14) defines a law of development of the system in time, and for its calculation it is sufficient to know only the Lagrange function (putting it differently, knowing the function (12), we can find  $\hat{H}$ ). The advantage of this method of quantization is that it is valid in any coordinate system and automatically gives the correct order of the operators in the Hamiltonian (see Ref. 1, p. 186 of the translation). Moreover, it can be readily generalized to the case of a curved space.<sup>6</sup> It is very probable that (12) is the correct quantization prescription in spaces with



curvature. Of course, it is desirable to have independent confirmation of this. Unfortunately, the simplest model (particle in the layer between two concentric spheres when the thickness of the layer tends to zero) does not give a unique answer.<sup>18</sup> Evidently, ellipsoids should be taken instead of spheres.

### The Feynman-Pauli Criterion

With regard to Eq. (16), Feynman noted in passing that it is true only for potentials which increase not faster than the second power of  $q$  (see Ref. 1, p. 185 of the Russian translation). Pauli<sup>4</sup> paid more attention to this question, giving, in particular, a concrete example of the insufficiency of Eqs. (16) and (12) [a particle in a box, for which the potentials is given by  $V(q) = (2|q - L/2|/L)^\alpha$ , i.e., it increases faster than any power of  $q$ ; see Sec. 1]. An extensive investigation of this problem has been published by Choquard.<sup>79</sup>

The essence of the problem is as follows. As was emphasized in Sec. 1, in the expressions characteristic of path integrals of the type

$$\Psi_\varepsilon(q) \approx \int_{-\infty}^{\infty} \frac{dq'}{(2\pi i \hbar)^{n/2}} \exp \left\{ \frac{i}{\hbar} \left[ \frac{(q - q')^2}{2\varepsilon} - \varepsilon V(q') \right] \right\} \Psi_0(q'), \quad \varepsilon \rightarrow 0, \quad (181)$$

it is necessary to retain the terms of order  $\varepsilon$ . Therefore, the value of the path integral is entirely determined by the asymptotic behavior of the expression (181), which can be found by the method of stationary phase.<sup>54</sup> The principal term in the argument of the exponential is traditionally assumed to be  $\Delta q^2/\varepsilon$ . This is indeed the case for potentials which increase at infinity not faster than  $q^2$ . However, for more rapidly growing potentials the term  $\varepsilon V(q')$  can no longer be ignored at large  $q'$  compared with  $\Delta q^2/\varepsilon$ . We illustrate this by the example of the potential  $V(q) = \lambda q^k$  in one-dimensional space ( $n=1$ ). To find the asymptotic behavior of such integrals, we use the following method.<sup>7)</sup> In (181), we go over to the new variables  $q = y/\varepsilon^\alpha$ ,  $q' = y'/\varepsilon^\alpha$ , finding  $\alpha$  from the condition of equality of the powers of  $\varepsilon$  in the two terms in the square brackets, i.e., from the equation  $1/\varepsilon^{1+2\alpha} = \varepsilon^{1-\alpha k}$ :

$$\alpha = 2/(k-2). \quad (182)$$

Equation (181) takes the form

$$\Psi_\varepsilon(y/\varepsilon^\alpha) \approx \frac{1}{\varepsilon^\alpha} \int_{-\infty}^{\infty} \frac{dy'}{(2\pi i \hbar)^{1/2}} \times \exp \left\{ \frac{i}{\hbar} \frac{1}{\varepsilon^{2\alpha+1}} \left[ \frac{(y - y')^2}{2} - \lambda y'^k \right] \right\} \Psi_0(y'/\varepsilon^\alpha). \quad (183)$$

Since  $2\alpha+1 > 0$  for  $k > 2$ , the asymptotic behavior of the integral (183) is found by the standard method. We obtain the stationary points of the argument of the exponential from the equation

$$y' - y - k\lambda y'^{k-1} = 0, \quad (184)$$

which has  $k-1$  solutions. One of them can be calculated for  $y \rightarrow 0$  [as  $\varepsilon \rightarrow 0$  and for fixed  $q$  we have  $y = O(\varepsilon^\alpha)$ ] by perturbation theory:

$$y'_0 \approx y + k\lambda y^{k-1}, \quad (185)$$

<sup>7)</sup> I am grateful to S. Yu. Slavyanov for pointing out this device to me.

and it corresponds to the assumption that  $\Delta q^2/\varepsilon$  is the leading term. The remaining solutions are not small. They make a contribution of the form

$$\sum_m c_m \exp(iA_m/\hbar \varepsilon^{2\alpha+1}) \Psi_0(y'_m/\varepsilon^\alpha), \quad (186)$$

where  $y'_m$  is the root of Eq. (184) with the number  $m$ , and the coefficient  $A_m$  is equal to  $(y - y'_m)^2/2 - \lambda y'^k$ . Similar expressions are obtained in the case of integration in (181) over a finite or semi-infinite interval. For finite intervals, the amplitude  $\psi_0$  is taken at a point of the boundary; here, the asymptotic behavior of (186) in the limit  $\varepsilon \rightarrow 0$  is determined by the behavior of  $\psi_0$  at infinity. It is clear that for sufficiently rapidly decreasing functions  $\psi_0 \sim 1/q^{(1/\alpha+\delta)}$ ,  $\delta > 0$  the contribution of the remaining stationary points can be ignored. If their contribution is to be ignorable in the path integral as well, we require as rapid a decrease of  $\psi_0$  at finite  $t$ . For states with finite energy (even  $k$ )  $\psi \sim 1/q^{(k+1+2\delta)/2}$ ,  $\delta > 0$ , and  $(k+1+2\delta)/2 > 1/\alpha + \delta = (k-2)/2 + \delta$ , i.e., this condition is always satisfied.

Choquard<sup>79</sup> investigated the contributions to the asymptotic behavior of (181) from paths joining the points  $q(0)$  and  $q(t)$ . For potentials of the type  $V = q^{2k}$ , there is not only the main path but also reflected paths that possess extremal properties. The conclusion drawn in Ref. 79 is that for sufficiently short times the contribution of the reflected paths can be ignored.

### Other definitions of path integrals

It is sometimes asserted (see, for example, Ref. 62, p. 60) that the nonuniqueness of the path integrals noted in Refs. 30 and 52 is indicative of a defect in their definition as limits of multiple integrals. Partly for this reason attempts have been (and are being) made to find an independent definition of path integrals. One such proposal reduces to defining them as entities possessing only those properties inherent in the simplest ( $g_{ij} = \text{const}$ ) Gaussian integrals.<sup>76, 80, 81</sup> We first emphasize the value of looking for other definitions of path integrals<sup>45</sup>—it is obviously necessary to have a better or, at least, more fully developed formalism. However, we also note the following. The nonunique features associated with path integrals have a dual nature. First, they reflect the dependence of the result on the order of the operators. But this is by no means a shortcoming. It is insensitivity of limits of the type (4) and (75) to the order of the operators that should be recognized as a shortcoming. Second, expressions of the type (5) and (75) do not define the integral uniquely (see Secs. 1 and 2). This second nonuniqueness is also not a shortcoming of the entity itself (the path integral defined by a limiting process from an integral of finite multiplicity) but a shortcoming of the notation. As was explained in Secs. 1 and 2, Eqs. (5) and (75) must be augmented by a symbol indicating the point at which the functions are taken in the prelimit formula. Then the path integrals written down formally become well-defined. A similar situation obtains with singular integrals of the type  $\int dx/x$ . To give them a meaning, it is necessary to specify what is understood by the given symbols, augmenting them by an appropriate symbol, say the letter  $P$  in front of the integral. Thus, if the problem is

posed physically, i.e., we are given the Lagrange function or the Hamilton operator, then, using the results of Secs. 1 or 2, we can uniquely construct a path integral in conformity with the postulates of quantization and the laws of quantum mechanics.

Finally, some words concerning their definition as entities endowed solely with the properties of Gaussian integrals. Since the integrals with  $g_{ij} \neq \text{const}$  differ strongly from ordinary Gaussian integrals (the need for the introduction of the symbol  $\alpha$ , etc.; see Secs. 1 and 2), such a definition applies only to a small class of objects; this is the first comment. Second, as a consequence, the class of operations that one can perform when working with such integrals is too small, since a nonlinear change of variables does not even belong to the class of admissible operations. With regard to the situation in field theories, see below.

### Path integrals in quantum field theory<sup>82,83</sup>

Although the present paper has been devoted to non-relativistic quantum mechanics, its final goal is quantum field theory. This theory is complicated in itself, and it is therefore natural to want to study the individual features of it that are associated with path integrals in simpler models. The most important matters discussed above (the nonstandard terms and the equivalence rules) are retained in quantum field theory, albeit in a modified form. A difference is that the commutator of the canonical variables now contains a  $\delta$  function:  $[\hat{\phi}(\mathbf{x}, t), \hat{\pi}(\mathbf{x}', t)] = i\hbar\delta(\mathbf{x} - \mathbf{x}')$ . But the equivalence rules are essentially a method for taking into account the noncommutativity of the operators, since the appearance of terms in  $A^{\text{eff}}$  and  $V^{\text{eff}}$  proportional to  $\hbar$  and  $\hbar^2$  is due to the actual use of commutation relations. Therefore, allowance for the extraterms is associated here with the appearance in  $H_{\text{int}}^{\text{eff}}$  of singular terms of the type  $\hbar\delta^{(3)}(0)$  and  $[\hbar\delta^{(3)}(0)]^2$ . Such corrections were encountered in the study of systems containing second derivatives in the interaction.<sup>84,85,16,17</sup> In Ref. 85, in which chiral theory is considered as an example, it is shown that one must take into account the terms proportional to  $[\hbar\delta^{(3)}(0)]^2$  in  $H_{\text{int}}^{\text{eff}}$  (the  $S$  matrix is defined as a Wick time-ordered product:  $S = T^*\{\exp[-(i/\hbar) \int d^4x \hat{H}_{\text{int}}^{\text{eff}}]\}$ )—their contribution cancels against the corresponding terms which arise in the diagrams with more than one loop. The use of the relativistically invariant dimensional regularization obviously makes it unnecessary to take them into account.<sup>17</sup>

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## APPENDIX 1

### 1. Curvilinear coordinates

It is easy to show that in curvilinear coordinates the well-known formulas of quantum mechanics are changed as follows. The scalar product becomes

$$\langle \Psi_1 | \Psi_2 \rangle = \langle \Psi_1 | q \rangle \langle q | \Psi_2 \rangle = \int d^n q \sqrt{g} \Psi_1^*(q) \Psi_2(q); \quad (\text{A.1})$$

the momentum operators become

$$\hat{P}_j = \frac{\hbar}{i} g^{1/4} \frac{\partial}{\partial q^j} g^{1/4}; \quad [\hat{q}^i, \hat{P}_j] = i\hbar \delta_j^i. \quad (\text{A.2})$$

These operators are Hermitian if the scalar product of the vectors of the Hilbert space are defined in accordance with (A.1). Their eigenfunctions are

$$\langle q | p \rangle = \frac{1}{(2\pi\hbar)^{n/2}} g^{-1/4} \exp(i p_j q^j / \hbar). \quad (\text{A.3})$$

and the  $\delta$  function is given by

$$\langle g | p \rangle \langle p | q' \rangle = (g g')^{-1/4} \delta^{(n)}(q - q') \equiv \delta(q, q'). \quad (\text{A.4})$$

The Laplace-Beltrami operator becomes

$$\square = \frac{1}{\sqrt{g}} \frac{\partial}{\partial q^i} \sqrt{g} g^{ij} \frac{\partial}{\partial q^j} = -\frac{1}{\hbar^2} g^{-1/4} \hat{P}_i g^{1/2} g^{ij} \hat{P}_j g^{-1/4}. \quad (\text{A.5})$$

If in (A.1) we integrate from  $-\infty$  to  $+\infty$ , then the operators (A.2) are self-adjoint. In Ref. 6, the more general case when the metric tensor depends on the time is considered.

If  $g \neq 1$ , then the kernels of the operators are modified as follows. Suppose an arbitrary operator  $F(\hat{q}, \hat{p})$  is given. We go over to the operator ordered in the standard manner:  $F(\hat{q}, \hat{p}) = F^s(\hat{q}, \hat{p})$ . Then the kernel of  $\hat{F}^s$  can be represented in the form

$$\langle q | F^s(\hat{q}, \hat{p}) | q' \rangle = \int d\tilde{p} \langle q | p \rangle F^s(q, p) \langle p | q' \rangle. \quad (\text{A.6})$$

Since  $\langle q | p \rangle \rightarrow \langle q | \tilde{p} \rangle = g^{-1/4} \langle q | p \rangle$  for  $g \neq 1$ , the kernels of all the operators acquire the factor  $(g g')^{-1/4}$ , where  $g' = g(q')$ . The factor  $(g g')^{-1/4}$  can be eliminated by going over to the functions  $\tilde{\psi} = g^{1/4} \psi$  and the kernels  $\tilde{U}_{qq'} = (g g')^{1/4} U_{qq'}$ ; in this case, the factors  $\sqrt{g}$  multiplying  $dq$  disappear in all the formulas,

$$\int d\tilde{q} \tilde{\psi}_1^* \tilde{\psi}_2 = \int dq \tilde{\psi}_1^* \tilde{\psi}_2, \quad \tilde{\psi}_e(q) = \int dq' \tilde{U}_{qq'} \tilde{\psi}_e(q'). \quad (\text{A.7})$$

and the operator  $\hat{P}_j$  (A.2) becomes the ordinary operator:

$$\int \sqrt{g} dq \tilde{\psi}_1^* \hat{P}_j \tilde{\psi}_2 = \int dq \tilde{\psi}_1^* \frac{\hbar}{i} \frac{\partial}{\partial q^j} \tilde{\psi}_2. \quad (\text{A.8})$$

In the space of the functions  $\tilde{\psi}$  the operator  $H(\hat{q}, \hat{p})$  is transformed into

$$q^{1/4} H(\hat{q}, \hat{p}) g^{-1/4} = H(q, -i\hbar \partial / \partial q).$$

In the paper, we use the following notation:

for the Christoffel symbol

$$[ij, k] = (g_{ih, j} + g_{jh, i} - g_{ij, h})/2, \quad (\text{A.9})$$

for the Riemann-Christoffel tensor

$$R_{ijkl} = (g_{ij, kl} - g_{il, kj} - g_{kh, ij} + g_{kh, li})/2 + g^{mn}([ij, m][kl, n] - [kj, m][il, n]), \quad (\text{A.10})$$

for the Ricci tensor and the scalar curvature

$$R_{ij} = g^{kl} R_{iklj}; \quad R = g^{ij} R_{ij} \quad (\text{A.11})$$

( $R > 0$  for a sphere in three-dimensional Euclidean space).

### 2. Derivation of Eq. (19)

Differentiating the obvious equation

$$\int_{-\infty}^{\infty} \frac{d^n \Delta}{(2\pi i \epsilon \hbar)^{n/2}} \exp\left(\frac{i}{\hbar} g_{ij} \frac{\Delta^i \Delta^j}{2\epsilon}\right) = g^{-1/2} \quad (\text{A.12})$$

with respect to  $g_{ij}$  using the formula

$$dg = g g^{ij} dg_{ij}, \quad (A.13)$$

which follows directly from the relation  $\ln \det \hat{A} = \text{tr} \ln \hat{A}$ , we have

$$\int_{-\infty}^{\infty} \frac{d^n \Delta \Lambda^k \Delta^l}{(2\pi i \epsilon \hbar)^{n/2}} \exp \left( \frac{i}{\hbar} g_{ij} \frac{\Delta^i \Lambda^j}{2\epsilon} \right) = g^{-1/2} g^{kl} (i\epsilon \hbar). \quad (A.14)$$

Repeated differentiation with respect to  $g_{ij}$  with allowance for the equation

$$dg^{ij} = -g^{ik} g^{jl} dg_{kl}, \quad (A.15)$$

which follows from the trivial identity  $d(g^{ik} g_{kj}) = 0$ , gives

$$\int_{-\infty}^{\infty} \frac{d^n \Delta \Lambda^{j_1} \dots \Lambda^{j_{2k}}}{(2\pi i \epsilon \hbar)^{n/2}} \exp \left( \frac{i}{\hbar} g_{ij} \frac{\Delta^i \Lambda^j}{2\epsilon} \right) = g^{-1/2} (i\epsilon \hbar)^k [g^{j_1 j_2} \dots g^{j_{2k-1} j_{2k}} - \text{perm.}]_{(2k-1)!!}, \quad (A.16)$$

which is equivalent to Eq. (19) when (A.12) is taken into account. In the square brackets, we have here the sum of all possible different products of  $k$  tensors  $g^{ij}$ , in all  $(2k)!/(k!2^k) = (2k-1)!!$  terms.

## APPENDIX 2

### Determination of the pre-exponential factor in Eq. (12)<sup>7</sup>

We consider an ensemble of particles distributed with constant density in the phase space. Then the number of particles in an infinitesimal element of the phase space is

$$dN = C dp' dq', \quad C = \text{const.} \quad (A.17)$$

The number of particles at time  $t'$  in the volume  $dq'$  and at time  $t$  in the volume  $dq$  is given by

$$dN = C \det \left| \frac{\partial p'}{\partial q} \right| dq dq', \quad (A.18)$$

where  $p'$  in accordance with (136) is  $p'_i = -\partial S(q, q')/\partial q'^i$ , since the transition  $q', p' \rightarrow q, p$  is a canonical transformation with generating function  $S(q, q') = -F_1(q', q)$ .

In the quantum-mechanical description of this problem, we split the space into cells  $\Delta q'$  and, assuming that in each cell there is one particle, we obtain

$$\Psi_t(q) = \int U_{qq'} \Psi_{t'}(q') \sqrt{g'} dq' \approx U_{qq'} \Psi_{t'}(q') \sqrt{g'} \Delta q'. \quad (A.19)$$

It is assumed that the wave function is concentrated entirely within the cell and that the cell is sufficiently small. Using the normalization condition

$$\int |\Psi_{t'}(q')|^2 \sqrt{g'} dq' \approx |\Psi_{t'}(q')|^2 \sqrt{g'} \Delta q' = 1, \quad (A.20)$$

and taking into account (A.19), we obtain

$$dN = |\Psi_t(q)|^2 \sqrt{g} \Delta q = |\Psi_{t'}(q')|^2 \sqrt{g} \Delta q \sqrt{g'} \Delta q'. \quad (A.21)$$

Comparing (A.18) with (A.21), we conclude that

$$(g g')^{1/2} |U_{qq'}|^2 = |c|^2 \det | -\partial^2 S / \partial q^j \partial q'^i | = |c|^2 D, \quad (A.22)$$

where  $c$  is a constant, i.e.,  $|U_{qq'}| = |c| D^{1/2} (g g')^{-1/4}$ .

The constant  $c$  can be determined from the condition  $U_{qq'}(\epsilon) \rightarrow \delta(q, q')$  as  $\epsilon \rightarrow 0$  (see Refs. 5 and 8) and is equal to  $(2\pi i \hbar)^{-n/2}$ .

## APPENDIX 3

### 1. Derivation of the Schrodinger Equation<sup>4,6</sup>

We shall find the equation that the kernel (12) satisfies if the Lagrangian has the form (9). We require the Hamilton-Jacobi equation<sup>61</sup>

$$\partial S / \partial t + H(\partial S / \partial q, q) = 0, \quad (A.23)$$

where

$$H = g^{ij} (p_i - A_i) (p_j - A_j) / 2 + V, \quad (A.24)$$

and the conservation law

$$\frac{\partial D}{\partial t} + \frac{\partial}{\partial q^i} \left[ g^{ij} \left( \frac{\partial S}{\partial q^j} - A_j \right) D \right] = 0. \quad (A.25)$$

The derivation of Eq. (A.25) is elementary. We denote

$$\Phi_{ij} = \frac{\partial^2 S(q, q')}{\partial q^i \partial q'^j}; \quad \Phi^{jk} \Phi_{kl} = \Phi^{kj} \Phi_{li} = \delta_i^j \quad (\Phi_{ij} \neq \Phi_{ji}). \quad (A.26)$$

Since  $D = \det | -\Phi_{ij} |$ , it follows from the identity  $\ln \det \varphi = \text{Tr} \ln \varphi$  that

$$\partial D / \partial t = D \Phi^{ij} \partial \Phi_{ij} / \partial t; \quad \partial D / \partial q^k = D \Phi^{ij} \partial \Phi_{ij} / \partial q^k. \quad (A.27)$$

Applying to Eq. (A.23) the operator  $\partial^2 / \partial q^i \partial q'^j$ , multiplying it by  $\Phi^{ji}$ , and contracting, we obtain Eq. (A.25) after using (A.26) and (A.27). To derive the Schrödinger equation, we use the relations

$$\frac{\hbar}{i} \frac{\partial U}{\partial t} = \left[ \frac{\partial S}{\partial t} + \frac{1}{2} \frac{\hbar}{i} \frac{1}{D} \frac{\partial D}{\partial t} \right] U; \quad (A.28)$$

$$\left( \frac{\hbar}{i} \frac{\partial}{\partial q^j} - A_j \right) U = \left[ \frac{\partial S}{\partial q^j} - A_j + \frac{\hbar}{2i} \frac{1}{D g^{-1/2}} \frac{\partial}{\partial q^j} (D g^{-1/2}) \right] U; \quad (A.29)$$

$$\frac{1}{2 \sqrt{g}} \left( \frac{\hbar}{i} \frac{\partial}{\partial q^i} - A_i \right) \sqrt{g} g^{ij} \left( \frac{\hbar}{i} \frac{\partial}{\partial q^j} - A_j \right) U = \frac{1}{2} g^{ij} [ |i| |j| + \frac{\hbar}{2i \sqrt{g}} \frac{\partial}{\partial q^i} \{ \sqrt{g} g^{ij} |j| \} ] U, \quad (A.30)$$

where  $U$  is given by Eq. (12) and  $[ ]$  denotes the expression in the square brackets in (A.29). Adding now the left- and right-hand sides of Eqs. (A.28) and (A.30) and adding to both sides the term  $VU$ , we find [noting that on the right the terms which do not contain  $\hbar$  and are linear in  $\hbar$  cancel when allowance is made for (A.23) and (A.25), respectively]

$$\left( \frac{\hbar}{i} \frac{\partial}{\partial t} + \hat{H} \right) U = - \frac{\hbar^2}{2} \frac{1}{\sqrt{D g^{-1/2}}} \square \sqrt{D g^{-1/2}} U, \quad (A.31)$$

where

$$\hat{H} = \frac{1}{2 \sqrt{g}} \left( \frac{\hbar}{i} \frac{\partial}{\partial q^i} - A_i \right) \sqrt{g} g^{ij} \left( \frac{\hbar}{i} \frac{\partial}{\partial q^j} - A_j \right) + V. \quad (A.32)$$

Pauli<sup>4</sup> calls the terms on the right-hand side of (A.31) proportional to  $\hbar^2$  the "false terms," using, however, quotation marks. They can be readily calculated explicitly. Using Eqs. (A.44) and (A.5) and ignoring the terms  $O(\Delta)$ , we find that (A.31) can be written in the form

$$\left( \frac{\hbar}{i} \frac{\partial}{\partial t} + \hat{H} \right) U = - \frac{\hbar^2 R}{12} U. \quad (A.33)$$

### 2. Calculations of the action (14)

It is necessary to substitute into the integral (13) the solution of equations of motion for the Lagrangian (9),

$$g_{ij} \ddot{q}^j + [j, k, i] \dot{q}^j \dot{q}^k - F_{ij} \dot{q}^j + V, i = 0 \quad (F_{ij} = A_j, i = A_i, j), \quad (A.34)$$

the solution depending on the initial,  $q'$ , and final,  $q$ , values of the coordinates. We expand the solution  $q(t)$  in powers of  $\Delta = q - q'$ . For this, in accordance with the expansion

$$q(t) = q' + \dot{q}' t + \ddot{q}' t^2 / 2 + \ddot{\ddot{q}}' t^3 / 6 + \dots \quad (A.35)$$



we need to know the initial values of the time derivatives of  $q$  (up to the third order, it is found) in the form of series in powers of  $\Delta$ . Setting  $t = \varepsilon$  in (A.35), we obtain  $\dot{q}'_{(0)} = \Delta/\varepsilon$  in the lowest order in  $\Delta$ . To calculate  $\dot{q}'$  in the following orders, we need to know  $\ddot{q}', \ddot{q}'', \dots$ . From Eqs. (A.34), we find  $\ddot{q}$  as a function of  $\dot{q}$ . Then, differentiating (A.34) with respect to  $t$ , we find  $\ddot{q}'$  as a function of  $\ddot{q}$  and  $\dot{q}$  and hence, using once more the equations of motion, as a function of  $\dot{q}$ . If the values found for  $\ddot{q}(\dot{q})$  are substituted in (A.35), for  $t = \varepsilon$ , the result is a nonlinear relation of the form  $\dot{q}' = (q - q')/\varepsilon + f(\dot{q}', \varepsilon)$  which can be solved iteratively. We then have the following expressions for  $\dot{q}', \ddot{q}', \ddot{q}''$  (with the accuracy we require):

$$\dot{q}' \approx \frac{1}{\varepsilon} \left\{ \Delta^j + \frac{1}{2} g^{jn} [ik, n] \Delta^i \Delta^k + \frac{1}{3} ([ik, n], l - g^{mm'} [lk, m] [ln, m']) \Delta^i \Delta^k \Delta^l \right\} + \frac{1}{2} g^{ij} F_{ki} \Delta^k; \quad (\text{A.36})$$

$$\ddot{q}' \approx -\frac{1}{\varepsilon^2} g^{jk} [mn, k] \{ \Delta^m \Delta^n + g^{mm'} [il, m'] \Delta^i \Delta^l \Delta^n \} + g^{ij} F_{ik} \frac{\Delta^k}{\varepsilon}; \quad (\text{A.37})$$

$$\ddot{q}'' \approx -\frac{1}{\varepsilon^3} \{ g_{,l}^{jk} [mn, k] + g^{jk} [mn, l, k] - 2g^{jk} [in, k] g^{im'} [ml, m'] \} \Delta^m \Delta^n \Delta^l. \quad (\text{A.38})$$

All the functions on the right-hand sides of these expressions are taken at the point  $q'$ . Further, we have

$$S(q, q') = \int_0^\varepsilon L dt \approx L_0 \varepsilon + \frac{\varepsilon^2}{2} \frac{dL_0}{dt} + \frac{\varepsilon^3}{6} \frac{d^2 L_0}{dt^2}. \quad (\text{A.39})$$

Here,  $L_0, dL_0/dt, \dots$  denote the values of the Lagrangian and its total derivatives with respect to the time at  $t=0$ , calculated after substitution in  $L$  of the solution (A.35). It can be shown that the contribution from the last term in (A.39), which has the order  $\Delta^4/\varepsilon$ , is equal to zero, and the contribution from the second is  $(A_{m,n} - A^k [m, n, k]) \Delta^m \Delta^n / 2$ , which together with the contribution from the first term [it is readily calculated using (A.36)] gives the action (14) used in the text. This action can be obtained in a different way by solving the Hamilton-Jacobi equation (A.23).

### 3. Calculation of the determinant $D$

In accordance with the definition (A.26), we have, using (14),

$$\begin{aligned} \varphi_{ij} \approx & -\frac{1}{\varepsilon} \left\{ g_{ij} + [jk, i] \Delta^k + \frac{1}{6} [kl, i], j \right. \\ & + [jl, i], k + [jk, i], l - g^{mn} ([ij, m] [kl, n] \\ & \left. + [jk, m] [il, n]) + [jl, m] [ik, n] \right\} \Delta^k \Delta^l - \frac{\varepsilon}{2} F_{ij}; \end{aligned} \quad (\text{A.40})$$

(as always, we have written out only the important terms, and the  $q'$  appended to the curly brackets means that all the functions are taken at the point  $q'$ ). To calculate the determinant of the tensor  $-\varphi_{ij}$ , we use the operator formula<sup>6</sup>

$$\det(A+B) = \det A \left\{ 1 + \text{tr}(A^{-1}B) + \frac{1}{2} [\text{tr}(A^{-1}B)]^2 - \frac{1}{2} \text{tr}(A^{-1}BA^{-1}B) + \dots \right\}, \quad (\text{A.41})$$

and, applying it ( $A_{ij} \equiv g_{ij}/\varepsilon$ ), we obtain

$$\begin{aligned} D = & \frac{1}{\varepsilon^n} g' \left\{ 1 + \frac{1}{2\varepsilon} g_{,k} \Delta^k + \frac{1}{2} g^{ij} g^{mn} ([jk, i] [ml, n] \right. \\ & - [jk, m] [nl, i]) \Delta^k \Delta^l + \frac{1}{6} [g^{ij} (g_{ij, kl} + g_{il, kj} \\ & \left. - \frac{1}{2} g_{kl, ij}) - g^{ij} g^{mn} ([ij, m] [kl, n] + 2[ik, m] [jl, n])] \Delta^k \Delta^l \right\}. \end{aligned} \quad (\text{A.42})$$

Using the expansion

$$g^{1/2} \approx g'^{1/2} \left\{ 1 + \frac{1}{2\varepsilon} g_{,k} \Delta^k + \frac{1}{4} [g^{ij} g^{mn} (2[jk, i] [ml, n] - g_{jn, l} g_{im, k}) + g^{ij} g_{ij, kl}] \Delta^k \Delta^l \right\}_{q'}, \quad (\text{A.43})$$

we can represent the expression (A.42) in the form

$$D = \frac{(g g')^{1/2}}{\varepsilon^n} \left[ 1 + \frac{1}{6} R_{kl} \Delta^k \Delta^l \right], \quad (\text{A.44})$$

where  $R_{kl}$  is the Ricci tensor (A.9). The argument of the tensor in (A.44) is unimportant.

## APPENDIX 4

### 1. A different derivation of Eq. (69)

In the original formulation

$$\Psi_\varepsilon(r, \varphi) \approx \int_0^\infty \int_0^{2\pi} \frac{r' dr' d\varphi'}{2\pi i \varepsilon \hbar} \exp \left\{ \frac{i}{2\varepsilon \hbar} [r^2 + r'^2 - 2rr' \cos \Delta\varphi] \right\} \Psi_0(r', \varphi') \quad (\text{A.45})$$

we use the expansion<sup>86</sup>

$$\exp(-iz \cos \Delta\varphi) = \sum_{m=-\infty}^{\infty} J_m(z) \exp[i(\Delta\varphi + 3\pi/2)m] \quad (\text{A.46})$$

and replace the Bessel functions by their asymptotic behavior ( $|z| \rightarrow \infty$ ,  $|\arg z| < \pi$ )

$$J_m(z) = \sqrt{\frac{2}{\pi z}} \cos \left[ z - \left( m + \frac{1}{2} \right) \frac{\pi}{2} + \frac{m^2 - 1/4}{2z} \right] + O(z^{-3/2}); \quad (\text{A.47})$$

this representation is readily obtained from the general formula given in Ref. 86. Substituting (A.46) and (A.47) in (A.45) (and using the fact that  $z = rr'/\varepsilon \hbar$ ), we obtain

$$\begin{aligned} \Psi_\varepsilon(r, \varphi) \approx & \sum_{m=-\infty}^{\infty} \int_0^\infty \int_0^{2\pi} \frac{r' dr' d\varphi'}{2\pi i \varepsilon \hbar} \exp[i(r^2 + r'^2)/2\varepsilon \hbar] \left( \frac{i\varepsilon \hbar}{2\pi r r'} \right)^{1/2} \\ & \times \exp(im\Delta\varphi) \left\{ \exp \left[ -\frac{i}{\hbar} \left( \frac{r r'}{\varepsilon} + \varepsilon \frac{m^2 - 1/4}{2rr'} \hbar^2 \right) \right] \right. \\ & \left. - i(-1)^m \exp \left[ \frac{i}{\hbar} (\dots) \right] \right\} \Psi_0(r', \varphi'), \end{aligned}$$

whence, making a change of the variable of integration in the second term in the curly brackets,  $r' \rightarrow -r'$  we find

$$\begin{aligned} \Psi_\varepsilon(r, \varphi) \approx & \int_0^\infty \frac{r' dr'}{2\pi i \varepsilon \hbar} \sum_{m=-\infty}^{\infty} \int_0^{2\pi} d\varphi' \\ & \times \exp \left\{ \frac{i}{\hbar} \left[ m\hbar \Delta\varphi - \varepsilon \frac{(m\hbar)^2 - \hbar^2/4}{2r^2} + \frac{\Delta\varphi^2}{2\varepsilon} \right] \right\} \sqrt{\frac{i\varepsilon \hbar}{2\pi r r'}} \Psi_0(r', \varphi'). \end{aligned} \quad (\text{A.48})$$

Here, we have ignored the terms of order  $\varepsilon \Delta$ ;  $\Psi_0(r', \varphi')$  is defined as  $\psi_0(r', \varphi')$  for  $r' > 0$  and  $\psi_0(-r', \varphi' + \pi)$  for  $r' < 0$ . Now, using Eq. (117), we rewrite (A.48) in the form

$$\begin{aligned} \Psi_\varepsilon \approx & \int_0^\infty \frac{r' dr'}{2\pi i \varepsilon \hbar} \int_0^\infty \int_0^{2\pi} \frac{dp_\varphi d\varphi'}{\hbar} \sqrt{\frac{i\varepsilon \hbar}{2\pi r r'}} \\ & \times \exp \left\{ \frac{i}{\hbar} \left[ p_\varphi \Delta\varphi - \varepsilon \frac{p_\varphi^2}{2r^2} + \frac{\Delta\varphi^2}{2\varepsilon} + \frac{\varepsilon \hbar^2}{8r^2} \right] \right\} \Psi_0(r', \varphi'). \end{aligned} \quad (\text{A.49})$$

In (A.49), we have taken into account the periodicity of  $\Psi_0$  with respect to  $\varphi'$ . Integrating over  $p_\varphi$ , we arrive at Eq. (70). Thus, the transition to the limit  $\varepsilon \rightarrow 0$  after application of the expansion (A.46) preserves the periodicity of the kernel of the evolution operator.

### 2. The prescription of Ref. 73 as applied to the model in Sec. 4

We shall show that direct elimination of the unphysical variables in the Hamiltonian path integral by sub-

stitution in it of the corresponding  $\delta$  functions from the constraints leads to a different result from the postulate (163). In accordance with this prescription,<sup>73</sup>

$$\langle q | \hat{U}(t-t') | q' \rangle = \int \prod_t \frac{dq dp}{(2\pi\hbar)^{n-s}} \prod_s \delta(\varphi_s) \delta(\chi^s) \times \det \{ \chi^s, \varphi_s \} \exp \left\{ \frac{i}{\hbar} \int_{t'}^t [p_i \dot{q}^i - H(q, p)] dt \right\}, \quad (\text{A.50})$$

where  $\varphi_s$  are constraints of the first class;  $\chi^s$  are subsidiary conditions having the properties  $\{\chi^s, \chi^s\} = 0, \det\{\chi^s, \varphi_s\} \neq 0$ .

Applying (A.50) to the model considered in Sec. 4 (we take  $t - t' = \varepsilon \rightarrow 0$ ), we have

$$\bar{\Psi}_\varepsilon(r, q) \approx \int \frac{dp_r dp_\varphi dr'}{2\pi\hbar} \exp \left\{ \frac{i}{\hbar} \left[ p_r (r \cos \Delta_\varphi - r') + p_\varphi \frac{r}{r'} \sin \Delta_\varphi - \varepsilon \left( \frac{p_r^2}{2} + \frac{p_\varphi^2}{2r^2} + V \right) \right] \right\} \delta(\varphi') \delta(p_\varphi) \Psi_0(r', q'), \quad (\text{A.51})$$

where  $\Delta_\varphi = \varphi - \varphi'$ . In the integral (A.51), we have made a transition to a polar coordinate system:  $p_r = (p, n_r')$ ;  $p_\varphi = r'(p, n_\varphi')$ ;  $\mathbf{x} = r' \mathbf{n}_r'$ ,  $\mathbf{x} = r \mathbf{n}_r$ ;  $\mathbf{n}_r$  and  $\mathbf{n}_\varphi$  are unit vectors; as a subsidiary condition we have taken  $\chi = \varphi' = 0$  (the variables  $\gamma$  and  $\pi$  are eliminated—their presence changes nothing). If in (A.51) we integrate over  $\varphi'$  and  $p_\varphi$  and in the spirit of (A.50) set  $\varphi = 0$ , we obtain

$$\bar{\Psi}_\varepsilon(r) \approx \int \frac{dp_r dr'}{2\pi\hbar} \exp \left\{ \frac{i}{\hbar} \left[ p_r \Delta r - \varepsilon \left( \frac{1}{2} p_r^2 + V \right) \right] \right\} \Psi_0(r'). \quad (\text{A.52})$$

It is easy to show that  $\bar{\Psi}_\varepsilon$  satisfies the Schrödinger equation with the Hamiltonian (172), which differs from Eq. (169) for the physical wave functions.

## ADDENDUM

1. The device used in Appendix 4 admits generalization to the case of spherical coordinates in  $n$ -dimensional space. Then in the path integral the integration with respect to the radial variable, all the angular variables, and all the momenta is with infinite limits, and the rule for defining the wave function outside the physical region is obtained automatically during the process of derivation. This rule can also be specified by means of the operator  $Q$  (see Sec. 1), so that the final expressions have the form (51).

2. In the practically important case when the constraints of the first class form a Lie algebra (the constraints are linear in the momenta and coordinates) and if there is no ordering problem in the constraints, the explicit form of the Hamiltonian  $H_{\text{eff}}$  in Eq. (179) can be specified. Suppose the eliminated unphysical variables are  $q^s, p_s$ , the remaining physical variables  $q^r, p_r$ , and the solutions of the constraints  $\varphi_s = 0$  are  $p_s = f_{sr}(q) p_r$ . Suppose further that the solutions of the subsidiary conditions  $\chi^s(q) = 0$  are  $q^s = 0$  [the functions  $\chi^s$  do not depend on  $p$  and  $\{\chi^s, \varphi_s\} = \delta^s_s$ ]. Since  $f_{sr}|_{q^s=0} = 0$ , it would appear, because of the factor  $\Pi \delta(\chi) \delta(\varphi)$  in the integrand, that in the Hamiltonian we can simply set  $q^s = p_s = 0$ . In reality, the equation  $p_s = f_{sr}(q) p_r$  is satisfied only on the functions  $\psi_{\text{phys}}$ , and therefore the terms bilinear in the momenta are replaced in accordance with the rule

$$p_s p_{s'} = p_s f_{sr} p_r = -i\hbar \frac{\partial}{\partial q^s} f_{sr} p_r + f_{sr} p_s p_r \quad (\text{B.1})$$

and the term with the derivative does not vanish as  $q^s \rightarrow 0$ . With allowance for this circumstance, the Hamiltonian (80) is replaced by

$$\hat{H}_{\text{eff}}^s = \hat{H}^s - \frac{i\hbar}{2} g^{ss'} \frac{\partial f_{s'r}}{\partial q^s} \hat{p}_r. \quad (\text{B.2})$$

The Hamiltonian in (179) is obtained from  $\hat{H}_{\text{eff}}^s$  by going over to the antistandard ordering. If there is an ordering problem in the constraints,  $H_{\text{eff}}$  has a somewhat more complicated form, though in this case too explicit expressions can be written down.

3. The proof that the form of the Lagrangian and Hamiltonian equivalence rules are not changed when the point of expansion, i.e., the point at which the functions in Eqs. (22) and (84) are taken, is changed will be published separately (Vestn. Leningr. Univ.).

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