Progress of Theoretical Physics, Vol. 65, No. 1, January 1981

A Path Integral Formalism of Collective Motion

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(Received June 27, 1980)

A quantum mechanical formalism of collective motion is proposed by using the idea of path integral method. Time evolution of many-body system is described by the propagator which joins the many-body state vectors parametrized by complex collective parameters. A general form of path integral representation for the propagator is derived in the complex parameter space. In particular the case of the coherent state representation is discussed in detail. It is pointed out that the time-dependent variation principle and especially the time dependent Hartree-Fock are naturally obtained as a classical limit.

§ 1. Introduction

The microscopic theory of nuclear collective motion has renewed interests in relation to the large amplitude collective phenomena which are supposed to occur typically in fission or heavy ion collision. The most conventional approaches developed so far are known to be the time dependent Hartree-Fock (TDHF),[1)~3)] especially the adiabatic TDHF[2)] and the generator coordinate theory.[4)]

In this paper we put forward a different formalism of collective motions by using the idea of path integral method.[5)] The utility of path integrals for collective excitations of many fermion systems was suggested by using the functional integral over Grassmann numbers,[6)] but this seems to be as yet applicable only to schematic models. Apart from this, we shall develop a path integral theory of collective motion without using any special model.

As will be stated in the next section, the basic idea is the following: The time evolution of many-body systems is described by the transition amplitude (or propagator) which joins the sequence of many body state vectors parametrized by appropriate collective parameters. The collective parameters are in general assumed to be complex (§ 3). By assuming the parametrized family of state vectors to be the "generalized coherent state" and using the completeness relation holding for it, the propagator is cast into a path integral form in the complex parameter space.

Although to use the parametrized family of many-body state vectors is a key concept of the TDHF, the collective Hamiltonian derived from this parametrization is essentially of classical nature and is required to be quantized in order to be compared with experimental results such as energy spectra. However, the two step procedure such as requantization after derivation of classical Hamiltonian seems rather to be a detour. The path integral formalism presented here may be advantageous in the sense that without using the classical Hamiltonian the collective motion is quantized from the beginning and that as a classical limit the TDHF is naturally derived.

The contents of the paper are as follows: In the next section we introduce the propagator for the collective motion. In § 3 we derive a general form of the path integral representation of the propagator in the complex parameter space and show that the time-dependent variation principle is obtained as a classical limit. In § 4 we consider the coherent state representation as a special case of the parametrization; the propagator is reduced to the phase space path integral form and is converted into the Lagrangian form. We also derive the time dependent Schrödinger equation of collective motion. The last section gives some additional remarks.

§ 2. Basic idea

The path integral method, as is well known, enables us to formulate the quantum process in a space-time picture, which is closely connected with the concept of the trajectory (or path) of the corresponding classical system through the probability amplitude for the path. A merit of this formalism, as was emphasized by Feynman,[7] lies in the point that if one deals with interacting dynamical systems, e. g., electron-photon system in QED, electron-phonon system in solid state and the relative motion coupled with internal electronic motion in atomic collision, a part of the dynamical variables can be eliminated from the total system by constructing the "reduced propagator". For example, in the case of QED the longitudinal photon is eliminated and the static Coulomb potential emerges.

The above mentioned examples are the ones in which the degrees of freedom are exactly separated into two groups. In the nuclear collective motion the separation of degrees of freedom into collective and internal motions from the original many-body Hamiltonian is in general rather complicated except for special simple cases such as center-of-mass motion. Thus if one is concerned with the application of the path integral to the nuclear collective motion, it is desirable to find out the prescription so as to deduce directly the propagator for collective motion from the original many-body Hamiltonian without separating of degrees of freedom into collective and internal parts. In the following we shall realize this in a simple approximate manner. For this purpose we remember the idea of the reduced propagator which was introduced by Pechukas[8] for the relative motion in the atomic collision and take over this idea into the nuclear collective motion.

In the atomic collision, one considers the collision of two atoms in their center-of-mass frame. Let $\boldsymbol{r}$ be the relative coordinate vector between two atoms and ξ be the totality of internal coordinates. The Hamiltonian is splitted into kinetic energy of relative motion and the remains;

$$H=\boldsymbol{p}^2/2m+h(\boldsymbol{r},\xi), \tag{2·1}$$

where $h(\boldsymbol{r},\xi)$ is assumed to satisfy the boundary condition $\lim_{r\to\infty}h(\boldsymbol{r},\xi)=h_0(\xi)$; $h_0(\xi)$ is the internal Hamiltonian. Suppose that one is interested in a collision where the internal states of atoms change from α to β. To describe this collision Pechukas defined the "reduced propagator"

$$K_{\beta\alpha}(\boldsymbol{r}''t''|\boldsymbol{r}'t')=\iint d\xi''d\xi'\varphi_\beta^*(\xi'')K(\boldsymbol{r}''\xi''t''|\boldsymbol{r}'\xi't')\varphi_\alpha(\xi') \tag{2·2}$$

instead of the full propagator

$$K(\boldsymbol{r}''\xi''t''|\boldsymbol{r}'\xi't')=\langle\boldsymbol{r}''\xi''|\exp[-iH(t''-t')/\hbar]|\boldsymbol{r}'\xi'\rangle, \tag{2·3}$$

which describes the transition $(\boldsymbol{r}',\xi')\to(\boldsymbol{r}'',\xi'')$. From (2·2) he derived a path integral representation and in the classical limit obtained the classical equations for relative motion associated with a given quantum transition $\alpha\to\beta$.

A utility of the expression (2·2) lies in the fact that one can effectively extract the propagator depending only on the relative coordinates by eliminating the internal coordinates through integration over them. Keeping this in mind we turn to the many-body system. First we note that Eq. (2·2) itself cannot be directly applied to the nuclear collective motion since we cannot well define the internal state corresponding to $\varphi_\alpha(\xi)$ and the full propagator corresponding to (2·3). Therefore we shall define the propagator for the collective motion in the following way: We assume that the dynamics of many-body system is described in the "subspace of the Hilbert space of the many-body system" which consists of all state vectors $\varphi(x,\zeta)$ parametrized by the "collective parameters" ζ where x represents the totality of the particle coordinates. Here we assume that the collective parameters ζ have in general N components, i. e., $\zeta=(\zeta^1,\cdots,\zeta^N)$. The simplest example of such a subspace may be given by the set of determinantal wave function parametrized by deformation parameters. Now tracing the expression (2·2) we define the propagator for the collective motion

$$K(\zeta''t''|\zeta't')=\iint dx''dx'\varphi^*(x'',\zeta'')K(x''t''|x't')\varphi(x',\zeta'). \tag{2·4}$$

$K(x''t''|x't')$ is the propagator for the many-body system

$$K(x''t''|x't')=\langle x''|\exp[-iH(t''-t')/\hbar]|x'\rangle \tag{2·5}$$

with H being the original many-body Hamiltonian. Equation (2·4) can be considered, at first sight, as an analogy with the reduced propagator (2·2); it gives the propagator for the collective motion effectively by integrating over particle coordinates. However, there is an essential difference; in Eq. (2·2) the dependence on the relative coordinate (which plays a rôle of collective coordinates) comes from the full propagator (2·3), whereas in our case the time development of collective motion arises from the parametrized state vectors $\varphi(x, \zeta)$. In this way Eq. (2·4) can be regarded as a transformation from the propagator of the original many-body system to the one for the collective parameter space labelled by ζ. Keeping this in mind the propagator (2·4) can be effectively represented as

$$K(\zeta''t''|\zeta't')=\langle\zeta''|\exp[-i\hat{H}(t''-t')/\hbar]|\zeta'\rangle. \tag{2·6}$$

The ket $|\zeta\rangle$ is defined through

$$\langle\zeta''|\zeta'\rangle=\int\varphi^*(x,\zeta'')\varphi(x,\zeta')dx \tag{2·7}$$

and the effective collective Hamiltonian $\hat{H}$ is defined by

$$\langle\zeta''|\hat{H}|\zeta'\rangle=\iint\varphi^*(x'',\zeta'')\langle x''|H|x'\rangle\varphi(x',\zeta')dx'dx''\,. \tag{2·8}$$

§ 3. Path integral in the complex parameter space and its classical limit

Now, as is usually done in the path integral theory, if the "resolution of unity" holds, the propagator (2·6) could be identically written as a continual integral form

$$K(\zeta''t''|\zeta't')=\lim_{n\to\infty}\int\prod_{k=1}^{n-1}d\zeta_k\prod_{k=1}^{n}\langle\zeta_k|\exp[-i\hat{H}\varepsilon/\hbar]|\zeta_{k-1}\rangle,$$

where $\varepsilon=(t''-t')/n$ and $\zeta_n=\zeta''$, $\zeta_0=\zeta'$. However, this is not the case, since the resolution of unity does not hold because of the non-orthogonality of the set $\{|\zeta\rangle\}$. It may be overcome by extending the collective parameters, which are a priori regarded as real, to the "complex parameters". The complex representations are frequently used in various physical problems. The simplest one is the coherent state which is defined as an eigenstate of the boson annihilation operator. In nuclear theory the coherent state is utilized, for example, in the generator coordinate theory[9] and as a powerful device for the calculation of norm kernel in cluster problem.[10] The path integral in the coherent state representation was long ago pioneered by Klauder in relation to the quantized theory of Bose fields.[11] However we shall start with the more general representation, which may be called the "generalized coherent state", since we may encounter the problems which cannot be treated within the usual coherent state.

In the generalized coherent state we can demand the "resolution of unity"

$$\int |\zeta\rangle d\mu(\zeta)\langle\zeta| = 1\,. \tag{3·1}$$

Here $\zeta(=(\zeta^1, \cdots, \zeta^N))$ represents the point of the N-dimensional complex parameter space*) and the measure $d\mu(\zeta)$ is given by

$$d\mu(\zeta) = \rho(\zeta, \zeta^*)\prod_{\alpha=1}^{N} d\,\mathrm{Re}\,\zeta^\alpha d\,\mathrm{Im}\,\zeta^\alpha \tag{3·2}$$

with $\rho(\zeta, \zeta^*)$ being a weight function which can be determined by the geometrical structure of the complex parameter space.**) The relation (3·1), which reveals the so-called "overcompleteness" of the set $\{|\zeta\rangle\}$, is equivalent to the reproducing relation

$$f(\zeta) = \int \langle\zeta|\zeta'\rangle f(\zeta') d\mu(\zeta'), \tag{3·3}$$

where $f(\zeta) = \langle\zeta|f\rangle$ for arbitrary ket $|f\rangle$. Note that $|\langle\zeta|\zeta'\rangle| \leqq 1$ where the equality holds for $\zeta=\zeta'$. With this relation the overlap $\langle\zeta|\zeta'\rangle$ is the so-called Bergman kernel function***) and plays a rôle of the delta-function as is implied by (3·3).

Inserting the resolution of unity repeatedly the propagator in the complex parameter space is expressed as

$$K(\zeta'' t''|\zeta' t') = \lim_{n\to\infty}\int \prod_{k=1}^{n-1} d\mu(\zeta_k)\prod_{k=1}^{n}\langle\zeta_k|\exp[-i\hat{H}\varepsilon/\hbar]|\zeta_{k-1}\rangle. \tag{3·4}$$

Each factor of the integrand in (3·4) is approximated as

$$\langle\zeta_k|\exp[-i\hat{H}\varepsilon/\hbar]|\zeta_{k-1}\rangle \simeq \langle\zeta_k|1-\frac{i}{\hbar}\varepsilon\hat{H}|\zeta_{k-1}\rangle$$

*) As complex parameter spaces (and the corresponding generalized coherent states), we can choose a rather wide class of spaces according to the collective motions under consideration. However, in this section we do not restrict the discussion to a specific space.

**) The measure is assumed to be purely constructed from the geometric property of parameter spaces (i.e., the metric) and not to be determined by the dynamical informations through the Hamiltonian alone.

***) We remark that the conventional Bergman kernel $\mathcal{K}(\zeta, \zeta')$ (for example, see the definition of Bargmann's article[13]) does not satisfy the normalization $\mathcal{K}(\zeta, \zeta)=1$ and the reproducing relation reads

$$\tilde{f}(\zeta) = \int \mathcal{K}(\zeta, \zeta')\tilde{f}(\zeta')d\tilde{\mu}(\zeta'),$$

where $\tilde{f}(\zeta)$ is the entire analytic function and $d\tilde{\mu}(\zeta)$ denotes the Bergman measure. This relation is however verified to be equivalent to (3·3) by a simple transformation $\mathcal{K}(\zeta, \zeta')\to\mathcal{K}(\zeta, \zeta')/\{\mathcal{K}(\zeta, \zeta)\times\mathcal{K}(\zeta', \zeta')\}^{1/2}$ together with $\tilde{f}(\zeta)\to\tilde{f}(\zeta)/\{\mathcal{K}(\zeta, \zeta)\}^{1/2}$ and $d\tilde{\mu}(\zeta)\to\mathcal{K}(\zeta, \zeta)d\tilde{\mu}(\zeta)(\equiv\rho(\zeta, \zeta^*)\times\prod_{\alpha=1}^{N} d\,\mathrm{Re}\,\zeta^\alpha d\,\mathrm{Im}\,\zeta^\alpha)$.

$$=\langle\zeta_k|\zeta_{k-1}\rangle\left(1-\frac{i}{\hbar}\varepsilon\langle\zeta_k|\hat{H}|\zeta_{k-1}\rangle/\langle\zeta_k|\zeta_{k-1}\rangle\right)$$
$$\simeq\langle\zeta_k|\zeta_{k-1}\rangle\exp\left[-\frac{i}{\hbar}\varepsilon\langle\zeta_k|\hat{H}|\zeta_{k-1}\rangle/\langle\zeta_k|\zeta_{k-1}\rangle\right]. \tag{3·5}$$

The factor $\langle\zeta_k|\zeta_{k-1}\rangle$, which is the kernel function in small time interval, is identically written as

$$\langle\zeta_k|\zeta_{k-1}\rangle=\exp[\log \varkappa(\zeta_k, \zeta_k^*; \zeta_{k-1}, \zeta_{k-1}^*)], \tag{3·6}$$

where we use the notation $\langle\zeta_k|\zeta_{k-1}\rangle\equiv\varkappa(\zeta_k, \zeta_k^*; \zeta_{k-1}, \zeta_{k-1}^*)$ in order to emphasize the dependence of complex conjugate ζ_k^* and ζ_{k-1}^* besides ζ_k and ζ_{k-1}. Expanding $\varkappa$ around ζ_{k-1} and ζ_{k-1}^*, we have

$$\begin{aligned}\varkappa(\zeta_k, \zeta_k^*; \zeta_{k-1}, \zeta_{k-1}^*)\simeq 1&+\left.\frac{\partial\varkappa}{\partial\zeta_k}\right|_{\zeta_k=\zeta_{k-1}}(\zeta_k-\zeta_{k-1})\\&+\left.\frac{\partial\varkappa}{\partial\zeta_k^*}\right|_{\zeta_k^*=\zeta_{k-1}^*}(\zeta_k^*-\zeta_{k-1}^*)\\&+O(\zeta_k-\zeta_{k-1})^2.\end{aligned} \tag{3·7}$$

Using $\log(1+x)\simeq x$ for $|x|\ll 1$ we get

$$\langle\zeta_k|\zeta_{k-1}\rangle\simeq\exp\left[\frac{i}{\hbar}\left\{\frac{\hbar}{i}\left(\frac{\partial\varkappa}{\partial\zeta_k}\Delta\zeta_k+\frac{\partial\varkappa}{\partial\zeta_k^*}\Delta\zeta_k^*\right)\right\}\right], \tag{3·8}$$

where we put $\Delta\zeta_k=\zeta_k-\zeta_{k-1}$ and the factor $\hbar/i$ is introduced for later convenience. If we define the "velocity" as $\dot{\zeta}_k=\Delta\zeta_k/\varepsilon$, (3·8) becomes

$$\exp\left[\frac{i}{\hbar}\left\{\frac{\hbar}{i}\left(\frac{\partial\varkappa}{\partial\zeta_k}\dot{\zeta}_k+\frac{\partial\varkappa}{\partial\zeta_k^*}\dot{\zeta}_k^*\right)\varepsilon\right\}\right]. \tag{3·9}$$

We note that in the expansion (3·7) we have omitted the quadratic terms $\Delta\zeta_k^2$ etc. The reason for this is the following: We note that $\Delta\zeta_k$ can be regarded to be of order ε, i. e., $\dot{\zeta}_k$ is finite, hence $\Delta\zeta_k^2$ is of order ε^2 and we can neglect. Next, the Hamiltonian term in Eq. (3·5) is approximated as

$$-\frac{i}{\hbar}\varepsilon\langle\zeta_k|\hat{H}|\zeta_{k-1}\rangle/\langle\zeta_k|\zeta_{k-1}\rangle\to-\frac{i}{\hbar}\varepsilon\langle\zeta_k|\hat{H}|\zeta_k\rangle$$

because the remaining terms are of higher order in ε. Thus we finally get the path integral representation in the complex parameter space

$$K(\zeta''t''|\zeta't')=\lim_{n\to\infty}\int\prod_{k=1}^{n-1}d\mu(\zeta_k)$$
$$\times\exp\left[\frac{i}{\hbar}\varepsilon\left\{\sum_{k=1}^{n}\frac{\hbar}{i}\left(\frac{\partial\chi}{\partial\zeta_k}\dot{\zeta}_k+\frac{\partial\chi}{\partial\zeta_k^*}\dot{\zeta}_k^*\right)-\langle\zeta_k|\hat{H}|\zeta_k\rangle\right\}\right],\tag{3·10}$$

which is formally written as

$$K(\zeta''t''|\zeta't')=\int\mathcal{D}\mu[\zeta(t)]\exp[iS/\hbar].\tag{3·11}$$

Here the path measure is defined by

$$\mathcal{D}\mu[\zeta(t)]=\lim_{n\to\infty}\prod_{k=1}^{n-1}d\mu(\zeta_k).$$

S is the action functional; $S=\int\mathcal{L}\,dt$ and the Lagrangian is given by

$$\mathcal{L}=\frac{\hbar}{i}\left\{\frac{\partial\chi}{\partial\zeta}\bigg|_{\zeta=\zeta'}\dot{\zeta}+\frac{\partial\chi}{\partial\zeta^*}\bigg|_{\zeta^*=\zeta'^*}\dot{\zeta}^*\right\}-\langle\zeta|\hat{H}|\zeta\rangle.\tag{3·12}$$

It should be mentioned that the first term of (3·12), which may be called "canonical term", determines the geometric structure of the dynamics on the complex parameter space since the kernel function is closely connected with the geometry of the complex parameter space.[14]

Now, if we note that the canonical term in Eq. (3·12) can be expressed as $\langle\zeta(t)|\partial/\partial t|\zeta(t)\rangle$, the path integral (3·11) can be rewritten in an alternative form

$$K(\zeta''t''|\zeta't')=\int\exp\left[\frac{i}{\hbar}\int_{t'}^{t''}\langle\zeta(t)|i\hbar\frac{\partial}{\partial t}-\hat{H}|\zeta(t)\rangle dt\right]\mathcal{D}\mu[\zeta(t)].\tag{3·13}$$

In the classical limit ($\hbar\to 0$), the dominant contribution to the path integral comes from the path which makes the action functional stationary (stationary phase approximation), thus we get the variation equation

$$\delta\int_{t'}^{t''}\langle\zeta(t)|i\hbar\frac{\partial}{\partial t}-\hat{H}|\zeta(t)\rangle dt=0\,,\tag{3·14}$$

which leads to the Euler-Lagrange equation

$$\frac{d}{dt}\left(\frac{\partial\mathcal{L}}{\partial\dot{\zeta}}\right)-\frac{\partial\mathcal{L}}{\partial\zeta}=0\tag{3·15}$$

together with the complex conjugate. Equation (3·14) is of a similar form to the usual time-dependent variation principle. However, it should be noted that this variation equation holds only for the case that the parametrized set of state vectors forms the "overcomplete set" which is characterized by the relation (3·1). The conventional time-dependent variation principle leads to the exact Schrödinger equation which is just the quantum mechanical equation. In this viewpoint it is curious that the variation equation (3·14) is obtained as a classical limit. But this puzzle may be resolved by taking account of the following fact: The true meaning of Eq. (3·14) lies in the point that it describes the classical dynamics in the complex parameter space, which is given by (3·15). This feature is closely connected with the fact that the generalized coherent state is essentially of classical character.

In this way we may state that the TDHF theory, which is a special case of the variation principle (3·14), is essentially of classical nature and the present path integral formalism serves as an "ab initio" quantized theory of the TDHF. In fact as was pointed out in Ref. 20) the Slater determinant space is constructed as the coherent state for the unitary group and the complex parameter space is realized as the complex Grassmann manifold.

§ 4. Path integral in the coherent state representation

As a specific case of the general formalism of the previous section, we consider that the parametrized state vector is given by the coherent state.[11),12)] The kernel function is then given by the Gaussian form

$$\langle\zeta'|\zeta\rangle=\exp[\zeta\cdot\zeta'^*-|\zeta|^2/2-|\zeta'|^2/2], \tag{4·1}$$

where the product $\zeta\cdot\eta^*$ denotes the scalar product, i. e., $\zeta\cdot\eta^*=\sum_{\alpha=1}^{N}\zeta^\alpha\cdot\eta^{\alpha *}$. The parameter space is the N-dimensional complex space C^N and the measure is given by

$$d\mu(\zeta)=\prod_{\alpha=1}^{N}\frac{1}{\pi}d\,\mathrm{Re}\,\zeta^\alpha d\,\mathrm{Im}\,\zeta^\alpha\,, \tag{4·2}$$

namely, the weight function $\rho(\zeta,\zeta^*)=\pi^{-N}$.

4. 1. *Reduction to the phase space path integral*

Substituting Eq. (4·1) into Eq. (3·15) we get the Lagrangian

$$\mathcal{L}=\frac{i\hbar}{2}(\zeta^*\dot{\zeta}-\zeta\dot{\zeta}^*)-\mathcal{H}(\zeta,\zeta^*) \tag{4·3}$$

with $\mathcal{H}(\zeta,\zeta^*)=\langle\zeta|\hat{H}|\zeta\rangle$. The physical meaning of the complex parameter ζ becomes clearer when it is represented in a real form:

$$\zeta = \frac{1}{\sqrt{2\hbar}}(q + ip). \tag{4·4}$$

Here q and p are assumed to be identified with coordinates and conjugate momenta (q and p denote the N-dimensional vectors). This reflects that the coherent state $|\zeta\rangle$ represents the minimal wave packet the center of which is at q and p and hence we can write $|\zeta\rangle = |qp\rangle$. The Lagrangian (4·3) is then expressed in terms of q and p

$$\mathcal{L} = \frac{1}{2}(p\dot{q} - q\dot{p}) - \mathcal{H}(q, p). \tag{4·5}$$

It should be noted that Eq. (4·5) is different from the usual Lagrangian in phase space ($\mathcal{L} = p \cdot \dot{q} - \mathcal{H}$) by a total derivative $-1/2\,(d/dt)(pq)$. The path integral is thus cast into the form

$$\begin{aligned} K(\zeta'' t'' | \zeta' t') &\equiv K(q'' p'' t'' | q' p' t') \\ &= \exp[i(p'' q'' - p' q')/2\hbar] \int \exp\left[i/\hbar \int_{t'}^{t''} (p\dot{q} - \mathcal{H}) dt \right] \mathcal{D}[q(t), p(t)] \end{aligned} \tag{4·6}$$

with the path measure

$$\mathcal{D}[q(t), p(t)] = \lim_{n\to\infty} \prod_{k=1}^{n-1} dq_k dp_k / (2\pi\hbar)^N . \tag{4·7}$$

The phase factor in Eq. (4·6) arises from the total derivative in the Lagrangian. In the classical limit ($\hbar \to 0$), with the aid of the stationary phase approximation, we get the variation equation

$$\delta \int_{t'}^{t''} (p\dot{q} - \mathcal{H}) dt = 0 , \tag{4·8}$$

which leads to the canonical equations

$$\dot{q} = \frac{\partial \mathcal{H}}{\partial p}, \qquad \dot{p} = -\frac{\partial \mathcal{H}}{\partial q} . \tag{4·9}$$

If the momentum p is small,[*] the effective collective Hamiltonian can be expanded in power series of p:

$$\mathcal{H} = V(q) + \sum_\alpha c^\alpha p^\alpha + \frac{1}{2} \sum_{\alpha\beta} \mathcal{M}^{\alpha\beta} p^\alpha p^\beta + \cdots . \tag{4·10}$$

[*] This corresponds to the adiabatic assumption in the TDHF theory.

$V(q)$ can be regarded as a potential energy and expressed in terms of the parametrized wave function

$$V(q)=\int\varphi^{*}(x'', q)\langle x''|H|x'\rangle\varphi(x', q)dx'dx'' . \tag{4·11}$$

$\mathcal{M}^{\alpha\beta}$, which is regarded as the inverse of mass tensor, i. e., $\mathcal{M}^{\alpha\beta}=(M^{-1})^{\alpha\beta}$, is given by

$$\mathcal{M}^{\alpha\beta}=\frac{\partial^{2}}{\partial p^{\alpha}\partial p^{\beta}}\langle q, p|\hat{H}|q, p\rangle\Big|_{p=0} \tag{4·12}$$

and is apparently symmetric $\mathcal{M}^{\alpha\beta}=\mathcal{M}^{\beta\alpha}$.

The propagator (4·6) has the same form as the conventional phase space path integral[15)~17)] except for the extra phase factor. However there is an essential difference; in the latter case the propagator, which is written as $K(q''t''|q't')$, is subjected to the boundary conditions $q=q'$ at $t=t'$ and $q=q''$ at $t=t''$ and these are compatible with the canonical equations of motion. Whereas, in the propagator (4·6) one makes a simulteneous assignment of coordinates and momenta as the end conditions. This implies that the number of boundary conditions is redundant in comparison with the number of canonical equations. In this respect, $K(q''p''t''|q'p't')$ should be regarded as a transition amplitude between wave packet states $|q'p'\rangle$ and $|q''p''\rangle$. On the contrary $K(q''t''|q't')$ is considered as the transition amplitude between coordinate eigenstates.

In spite of this difference we can formally extract the phase space path integral from (4·6). For this purpose, we take a Fourier transform as follows:

$$K(q''\tfrac{q''}{2}t''|q'\tfrac{q'}{2}t')$$
$$=\int dp'dp''\exp[i(p''q''-p'q')/2\hbar]K(q''p''t''|q'p't'). \tag{4·13}$$

This is analogous to the transformation from the momentum space propagator $K(p''t''|p't')$ to the coordinate space propagator $K(q''t''|q't')$[16)] which corresponds to the canonical transformation $q\to p$, $p\to -q$. Thus we get

$$K(q''\tfrac{q''}{2}t''|q'\tfrac{q'}{2}t')=\lim_{n\to\infty}\int\cdots\int dp_0dp_1\cdots dp_ndq_1\cdots dq_{n-1}/(2\pi\hbar)^{nN}$$
$$\times\exp[i/\hbar\{\sum_{k=1}^{n}p_k(q_k-q_{k-1})-\mathcal{H}(q_k, p_k)\varepsilon\}], \tag{4·14}$$

where we put $p'=p_0$ and $p''=p_n$. Since the integrand in (4·14) does not contain p_0, the integration over p_0 is separated out and we get

$$K\left(q''\frac{q''}{2}t''\middle|q'\frac{q'}{2}t'\right)=V_0\lim_{n\to\infty}\int\cdots\int dp_1\cdots dp_n dq_1\cdots dq_{n-1}/(2\pi\hbar)^{nN}$$
$$\times\exp\left[i/\hbar\int_{t'}^{t''}(p\dot{q}-\mathcal{H})dt\right], \qquad (4\cdot15)$$

where $V_0(\equiv\int dp_0)$ is the volume of the momentum space. Except for the factor V_0, which is infinite, the expression (4·15) becomes just the usual phase space path integral. The factor V_0 can be eliminated by redefining the propagator through the normalization $K\to K/V_0$, since V_0 is a trivial multiple factor and does not play any physical rôle.

Here we make a remark on the meaning of transformation (4·13). We can regard Eq. (4·13) as a kind of the Wigner transform[18),*)]

$$U(x,x')=\frac{1}{2\pi\hbar}\int dp\,\exp[ip(x-x')/\hbar]F\left(p,\frac{x+x'}{2}\right), \qquad (4\cdot16)$$

where $U(x,x')$ is a non-local function and $F(p,(x+x')/2)$ is a function in the phase space. Thereby Eq. (4·13) implies the transformation of the propagator between the wave packet $|q'p'\rangle$ and $|q''p''\rangle$ to the one between the wave packet $|q'q'/2\rangle$ and $|q''q''/2\rangle$. The ket $|q\ q/2\rangle$ may be considered as a wave packet with the "mean position" q. Thus Eq.(4·15) should be understood as the propagator for the transition from the wave packet whose center is at q' to the one whose center is at q'' and should not be regarded as the propagator between the eigenstates $|q'\rangle$ and $|q''\rangle$.

4.2. *Conversion into the Lagrangian form*

The phase space path integral (4·15) can be readily converted into the Feynman (or Lagrangian) form if the collective coordinates are rectangular. This is performed by generalizing the procedure in Refs. 16) and 17) to the case of the system with non-constant mass tensor.

In order to achieve this, we restrict the collective Hamiltonian (4·10) up to second order in p

$$\mathcal{H}=\frac{1}{2}\sum_{\alpha\beta}p^\alpha(M^{-1})^{\alpha\beta}p^\beta+V(q), \qquad (4\cdot17)$$

where we omit the linear term in p since this can be eliminated by an appropriate canonical transformation. The action functional is thus given by

$$S=\lim_{n\to\infty}\sum_{k=1}^{n}\left\{\sum_\alpha p_k{}^\alpha\Delta q_k{}^\alpha-\frac{1}{2}\sum_{\alpha\beta}p_k{}^\alpha(M^{-1})_k{}^{\alpha\beta}p_k{}^\beta\varepsilon-V(\bar{q}_k)\varepsilon\right\}, \qquad (4\cdot18)$$

*) About the Wigner transform, we are indebted to Prof. Horiuchi.

where we put $q_k{}^\alpha - q_{k-1}^\alpha = \Delta q_k{}^\alpha$ and the value of the mass tensor and the potential is taken at the intermediate of $q_k{}^\alpha$ and q_{k-1}^α, say $\bar{q}_k$, i.e., $(M^{-1})_k{}^{\alpha\beta} \equiv M^{-1}(\bar{q}_k)$. Equation (4·18) can be diagonalized by the orthogonal transformation

$$p_k{}^\alpha = \sum_{\gamma=1}^{N} t_k{}^{\alpha\gamma} \hat{p}_k{}^\gamma \,, \tag{4·19}$$

where t_k is determined so as to satisfy

$$\sum_{\alpha\beta} (M^{-1})_k{}^{\alpha\beta} t_k{}^{\alpha\gamma} t_k{}^{\beta\delta} = \sum_{\alpha\beta} ({}^T t)_k{}^{\gamma\alpha} (M^{-1})_k{}^{\alpha\beta} t_k{}^{\beta\delta}$$
$$= (\hat{M}^{-1})_k{}^\gamma \delta_{\gamma\delta} \,. \tag{4·20}$$

Thus the integral with respect to momenta in (4·15) becomes

$$\exp\left[\frac{i}{2\hbar}\sum_{k=1}^{n}\sum_{\gamma=1}^{N}(\Delta\hat{q}_k{}^\gamma)^2/(M^{-1})_k{}^\gamma\varepsilon\right]$$
$$\times\int\exp\left[-\frac{i}{2\hbar}\sum_{k=1}^{n}\sum_{\gamma=1}^{N}(M^{-1})_k{}^\gamma(\hat{p}_k{}^\gamma - \Delta q_k{}^\gamma/(M^{-1})_k{}^\gamma\varepsilon)^2\varepsilon\right]$$
$$\times\prod_{k=1}^{n}\frac{\partial(p_k{}^1\cdots p_k{}^N)}{\partial(\hat{p}_k{}^1\cdots\hat{p}_k{}^N)}d\hat{p}_k{}^1\cdots d\hat{p}_k{}^N \tag{4·21}$$

with

$$\Delta\hat{q}_k{}^\gamma = \sum_\alpha ({}^T t)_k{}^{\gamma\alpha}\Delta q_k{}^\alpha \,. \tag{4·22}$$

Noting the Jacobian $=\det(t^{\alpha\beta})=1$ and performing the Gaussian integral, we get

$$\prod_{k=1}^{n}\left\{(2\pi)^{N/2}\left(\prod_{\gamma=1}^{N}\left(\frac{i}{\hbar}(\hat{M}^{-1})_k{}^\gamma\varepsilon\right)^{-1/2}\right\}\right.$$
$$\times\exp\left[\frac{i}{2\hbar}\sum_{k=1}^{n}\sum_{\gamma=1}^{N}(\Delta\hat{q}_k{}^\gamma)^2/(\hat{M}^{-1})_k{}^\gamma\varepsilon\right]. \tag{4·23}$$

Further, by using the relation

$$\prod_{k=1}^{n}(\hat{M}^{-1})_k{}^\gamma = \det(\hat{M}^{-1})_k = \det(M^{-1})_k \tag{4·24}$$

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*) This relation is derived as follows: (4·22) is written as $\Delta q_k{}^\gamma = ({}^T\Delta q_k \cdot t_k)^\gamma$ in a matrix notation and

$$\{(\hat{M}^{-1})_k{}^\gamma\}^{-1} = (\hat{M})_k{}^{\gamma\gamma} = ({}^T t\cdot M\cdot t)_k{}^{\gamma\gamma} = \sum_{\alpha\beta}({}^T t)_k{}^{\gamma\alpha} M_k{}^{\alpha\beta} t_k{}^{\beta\gamma}.$$

Hence we get

$$\sum_\gamma(\Delta\hat{q}_k{}^\gamma)^2/(\hat{M}^{-1})_k{}^\gamma = \sum_\gamma({}^T\Delta q_k\cdot t_k)^\gamma \hat{M}_k{}^{\gamma\gamma}({}^T t_k\cdot\Delta q_k)^\gamma$$
$$= ({}^T\Delta q_k\cdot M_k\cdot\Delta q_k) = \sum_{\alpha\beta}\Delta q_k{}^\alpha M_k{}^{\alpha\beta}\Delta q_k{}^\beta.$$

together with

$$\sum_{\gamma=1}^{N}(\Delta\hat{q}_k{}^\gamma)^2/(\hat{M}^{-1})_k{}^\gamma=\sum_{\alpha\beta}\Delta q_k{}^\alpha M_k{}^{\alpha\beta}\Delta q_k{}^\beta\,, \tag{4·25}$$

*)

we finally obtain the Lagrangian form

$$K(q''t''|q't')=\lim_{n\to\infty}\int\prod_{k=1}^{n}\left\{\left(\frac{-i}{2\pi\hbar\varepsilon}\right)^N \det M_k\right\}^{1/2}dq_k{}^1\cdots dq_k{}^N$$

$$\times\exp\left[\frac{i}{\hbar}\int_{t'}^{t''}\left\{\frac{1}{2}\sum\dot{q}^\alpha M^{\alpha\beta}\dot{q}^\beta-V(q)\right\}dt\right]. \tag{4·26}$$

4. 3. *Schrödinger equation for collective motion*

We can derive the Schrödinger equation for the collective motion starting with the propagator (4·26). First we note that Eq. (4·26) has the same form as the propagator for the curved space, namely the mass tensor is just the metric tensor. Although the general procedures for the derivation of the Schrödinger equation in the curved space have been discussed by many authors, these are mathematically complicated (for example, see Ref. 19)). The following derivation is simple and follows the standard technique by Feynman.

Let $\Phi(q,t)$ be the collective wave function. The time development of Φ is given by the integral equation

$$\Phi(q,t+\varepsilon)=\int K(q\ t+\varepsilon|q't)\Phi(q',t)dq'\,. \tag{4·27}$$

$K(qt+\varepsilon|q't)$ is the "short time" propagator and given by

$$\left\{\left(\frac{-i}{2\pi\hbar\varepsilon}\right)^N\det M(q')\right\}^{1/2}$$

$$\times\exp\left[\frac{i}{2\hbar\varepsilon}\sum_{\alpha\beta}M^{\alpha\beta}(\bar{q})(q^\alpha-q^{\alpha'})(q^\beta-q^{\beta'})-\frac{i\varepsilon}{\hbar}V(q')\right]. \tag{4·28}$$

Here we assume that the mass tensor takes the value at the center of initial and final positions q and q', i.e., $\bar{q}=(q+q')/2$ and as for the potential it takes the value at the initial position q' since the potential may not change appreciably in small time interval. In order to convert the integral equation into the differential equation we adopt the change of variable: $q^\alpha=q^\alpha$ and $\xi^\alpha=q^\alpha-q^{\alpha'}$. We note that ξ is of order $\sqrt{\varepsilon}$ (see Ref. 7)). Due to this the integrand in Eq. (4·27) is expanded in the Taylor series of ξ, which consists of the following three terms: First, $\Phi(q',t)$ is expanded up to second order

$$\Phi(q',t)\simeq\Phi(q,t)-\sum_\alpha\frac{\partial\Phi}{\partial q^\alpha}\xi^\alpha+\frac{1}{2}\sum_{\alpha\beta}\frac{\partial^2\Phi}{\partial q^\alpha\partial q^\beta}\xi^\alpha\xi^\beta\,. \tag{4·29}$$

Second, the mass tensor is expanded in lowest order

$$M^{\alpha\beta}(\bar{q})\simeq M^{\alpha\beta}(q)-\frac{1}{2}\sum_\gamma\frac{\partial M^{\alpha\beta}}{\partial q^\gamma}\xi^\gamma \tag{4·30}$$

and hence exponential term in (4·28) becomes

$$\exp\Big[\frac{i}{2\hbar\varepsilon}\sum_{\alpha\beta}M^{\alpha\beta}(q)\xi^\alpha\xi^\beta\Big]\exp\Big[-\frac{i}{4\hbar\varepsilon}\sum_{\alpha\beta\gamma}\frac{\partial M^{\alpha\beta}}{\partial q^\gamma}\xi^\alpha\xi^\beta\xi^\gamma\Big], \tag{4·31}$$

the second factor of which may be further expanded up to lowest order as

$$1-\frac{i}{4\hbar\varepsilon}\sum_{\alpha\beta\gamma}\frac{\partial M^{\alpha\beta}}{\partial q^\gamma}\xi^\alpha\xi^\beta\xi^\gamma\,.$$

Third, the normalization factor $[\det M(q')]^{1/2}$ is expanded as

$$\begin{aligned}[\det M(q')]^{1/2}&\equiv[\det M(q-\xi)]^{1/2}\\ &\simeq[\det M(q)]^{1/2}-\sum_\alpha\frac{\partial[\det M(q)]^{1/2}}{\partial q^\alpha}\xi^\alpha\,.\end{aligned} \tag{4·32}$$

Thus the integral equation (4·27) becomes

$$\begin{aligned}\Phi(q,t+\varepsilon)=&\int\exp\Big[\frac{i}{2\hbar\varepsilon}\sum_{\alpha\beta}M^{\alpha\beta}\xi^\alpha\xi^\beta\Big]\Big(1-\frac{i}{4\hbar\varepsilon}\sum_{\alpha\beta\gamma}\frac{\partial M^{\alpha\beta}}{\partial q^\gamma}\xi^\alpha\xi^\beta\xi^\gamma\Big)\\ &\times\exp[-i\varepsilon V/\hbar]\Big(\Phi(q,t)-\sum_\alpha\frac{\partial\Phi}{\partial q^\alpha}\xi^\alpha+\frac{1}{2}\sum_{\alpha\beta}\frac{\partial^2\Phi}{\partial q^\alpha\partial q^\beta}\xi^\alpha\xi^\beta\Big)\\ &\times(2\pi\hbar i)^{-N}\Big\{[\det M(q)]^{1/2}-\sum_\alpha\frac{\partial[\det M(q)]^{1/2}}{\partial q^\alpha}\xi^\alpha\Big\}d\xi^1\cdots d\xi^N\,.\end{aligned} \tag{4·33}$$

By carrying out the Gaussian integrals (see the Appendix) we get

$$\begin{aligned}\Phi(q,t+\varepsilon)=&\exp[-i\varepsilon V/\hbar]\Big[\Phi(q,t)+\frac{\hbar\varepsilon i}{2}\sum_{\alpha\beta}(M^{-1})^{\alpha\beta}\frac{\partial^2\Phi}{\partial q^\alpha\partial q^\beta}\\ &+\frac{\hbar\varepsilon i}{2}\Big\{(\det M)^{1/2}\sum_{\alpha\beta}\frac{\partial}{\partial q^\alpha}\Big((\det M)^{-1/2}(M^{-1})^{\alpha\beta}\Big)\frac{\partial\Phi}{\partial q^\beta}\\ &+(\det M)^{-1}\sum_{\alpha\beta}(M^{-1})^{\alpha\beta}\frac{\partial(\det M)^{1/2}}{\partial q^\beta}\frac{\partial\Phi}{\partial q^\alpha}\Big\}\Big].\end{aligned} \tag{4·34}$$

Noting the expansion $\exp[-i\varepsilon V/\hbar]\simeq1-i\varepsilon V/\hbar$, $\Phi(q,t+\varepsilon)\simeq\Phi(q,t)+\varepsilon(\partial\Phi/\partial t)$

and comparing the terms of first order in ε we finally obtain

$$i\hbar\frac{\partial\Phi}{\partial t}=\left[-\frac{\hbar^2}{2}(\det M)^{-1/2}\sum_{\alpha\beta}\frac{\partial}{\partial q^\alpha}\left\{(\det M)^{1/2}(M^{-1})^{\alpha\beta}\frac{\partial}{\partial q^\beta}\right\}+V(q)\right]\Phi$$
$$\equiv\left(-\frac{\hbar^2}{2}\Delta_2+V(q)\right)\Phi\,, \tag{4·35}$$

where we use the relation

$$(\det M)^{1/2}\sum_{\alpha\beta}\frac{\partial}{\partial q^\alpha}[(\det M)^{1/2}(M^{-1})^{\alpha\beta}]\frac{\partial\Phi}{\partial q^\beta}$$
$$+(\det M)^{-1}\sum_{\alpha\beta}(M^{-1})^{\alpha\beta}\frac{\partial(\det M)^{1/2}}{\partial q^\beta}\frac{\partial\Phi}{\partial q^\beta}$$
$$=(\det M)^{-1/2}\sum_{\alpha\beta}\frac{\partial}{\partial q^\alpha}[(\det M)^{1/2}(M^{-1})^{\alpha\beta}]\frac{\partial\Phi}{\partial q^\beta}\,.$$

Equation (4·35) is just the Schrödinger equation obtained from the Pauli quantization for the collective Hamiltonian (4·17). This also coincides with the Schrödinger equation in the curved space with the metric $M^{\alpha\beta}$ (Δ_2 becomes the Laplace-Beltrami operator corresponding to this metric) except for the additional term coming from the curvature of the curved space which is derived from the more refined Riemannian geometric technique.[19]

§ 5. Additional remarks

In this paper we have investigated the quantum mechanical formalism of collective motion by using the path integral in the complex parameter space through the generalized coherent state. Particularly we have analyzed the case of the parametrization by the ordinary coherent state.

Here we give the following remarks on the present formalism: (i) So far we have implicitly assumed that the number of parameters specifying the parametrized set of state vectors is finite. However, the infinite number parametrization is possible. As a specific example of such a case we can mention the system of Bose particles. In this case the parametrized state vector is given by the symmetrical product form; $\langle x_1\cdots x_A|\psi\rangle=\prod_{i=1}^{A}\psi(x_i)$, which is considered to be the coherent state by virtue of the condensed nature. If we consider the single particle wave function $\psi(x)$ as the relevant parameters, then the number of parameters is continuously infinite. By the resolution of unity holding for $|\psi\rangle$ we may get the path integral expression for the propagator $K(\psi''t''|\psi't')$ and hence as a classical limit obtain the non-linear Schrödinger-like equation. (ii) It is known that the generalized coherent state is closely connected with the unitary representation of arbitrary Lie groups.[21] The ordinary coherent state is an example in which the corresponding Lie group is the so-called Heisenberg-Weyl group. In this way the path integral in the generalized coherent state would provide with a powerful tool for the quantized theory of collective motions through the dynamical group exhibiting the symmetry inherent in the many-body system. For example, the path integral in the representation of $SU(2)$ coherent state,[22] which is the simplest non-abelian coherent state, may serve as a useful device for the quantized rotational motion.

Acknowledgments

The author would like to thank Dr. Tōru Suzuki for many useful discussions on the coherent state path integrals. He is also grateful to Dr. Y. Mizobuchi for his careful reading of the manuscript. The author wishes to thank Dr. A. Hayashi and Professor H. Horiuchi for their kind interests. This work was performed as a part of the annual research project on the "Large amplitude collective motion" organized by the Research Institute for Fundamental Physics, 1979.

Appendix

We list up the formulas of the Gaussian integrals and the derivative of determinants.

i) Gaussian integrals: We write

$$I_m{}^{\rho\sigma\cdots}=\int\exp\left[\frac{i}{2\hbar\varepsilon}\sum_{\alpha\beta}M^{\alpha\beta}\xi^\alpha\xi^\beta\right]\xi^\rho\xi^\sigma\cdots\prod_{k=1}^N d\xi^k, \qquad (\mathrm{A}\cdot 1)$$

where m denotes an even integer. I_0 is calculated as

$$I_0=(2\pi\hbar\varepsilon i)^{N/2}(\det M)^{-1/2}. \qquad (\mathrm{A}\cdot 2)$$

By differentiating (A·2) with respect to $M^{\alpha\beta}$ under the integral symbol, we get

$$\left.\begin{aligned}I_2{}^{\rho\sigma}&=(2\hbar\varepsilon/i)(2\pi\hbar\varepsilon i)^{N/2}\frac{\partial}{\partial M^{\rho\sigma}}(\det M)^{-1/2}\,,\\ I_4{}^{\rho\sigma\eta\omega}&=(2\hbar\varepsilon i)^2(2\pi\hbar\varepsilon i)^{N/2}\frac{\partial^2}{\partial M^{\rho\sigma}\partial M^{\eta\omega}}(\det M)^{-1/2}\end{aligned}\right\} \qquad (\mathrm{A}\cdot 3)$$

and so on.

ii) Derivative of determinants: Using the formula

$$\frac{\partial}{\partial M^{\alpha\beta}}(\det M)=\Delta^{\alpha\beta}, \tag{A·4}$$

where $\Delta^{\alpha\beta}$ is the cofactor of the element $M^{\alpha\beta}$ and $(M^{-1})^{\alpha\beta}=\Delta^{\alpha\beta}(\det M)^{-1}$, we get

$$\left.\begin{aligned}&\frac{\partial}{\partial M^{\alpha\beta}}(\det M)^{-1/2}=-\frac{1}{2}(\det M)^{-1/2}(M^{-1})^{\alpha\beta},\\&\frac{\partial^2}{\partial M^{\rho\sigma}\partial M^{\alpha\beta}}(\det M)^{-1/2}=-\frac{1}{2}\frac{\partial}{\partial M^{\rho\sigma}}\{(\det M)^{-1/2}(M^{-1})^{\alpha\beta}\}\end{aligned}\right\} \tag{A·5}$$

and so on.

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