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On the quantum mechanics of chiral dynamics

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Abstract. A quantum-mechanical model of chiral invariance is studied, with particular emphasis on problems relating to the order of noncommuting factors. The difficulties which arise from an incorrect use of the Lagrangian are discussed. Using the canonical approach it is shown that the requirement of chiral invariance suffices to remove all ambiguities in the Hamiltonian, which is then given in a form analogous to that of the Sugawara model. A review, often critical, is made of related discussions by other authors.

1. Introduction

This study arose out of an attempt to pursue the feasibility of using a chiral invariant theory as the starting point for the description of hadron dynamics. In particular, the chiral invariant interactions of a system of zero-mass pseudoscalar mesons provides a nontrivial example of what might be the basis of a realistic theory in which of course the chiral invariance would be broken, the mesons would have mass, and other particles would exist. As is well known this field-theoretic model for a chiral invariant theory has as its Lagrange density

$$\mathscr{L}(x) = \tfrac{1}{2}\partial_\mu \phi^i(x) g_{ij}(\phi(x)) \partial^\mu \phi^j(x). \tag{1.1}$$

Here $\phi^i(x)$ are the fields of the meson multiplet ($i = 1, 2, \ldots, n^2-1$) and g_{ij} is constructed from the fields by a prescription specified in terms of the transformation properties of the fields under the action of the chiral group $\mathrm{SU}(n)\times\mathrm{SU}(n)$. Thus if the generators of the group are written in the usual way as V^i, A^i, we would write

$$[V^i, \phi^j] = \mathrm{i} f^{ij}{}_k \phi^k \tag{1.2}$$

$$[A^i, \phi^j] = \mathrm{i} f^{ij}(\phi). \tag{1.3}$$

The fields transform under the adjoint representation of the parity conserving (diagonal) subgroup generated by V^i, but nonlinearly under chiral transformations. The nonlinear functions f^{ij} of the fields are not uniquely determined by the group law, but once they are given the 'metric tensor' g_{ij} is determined unambiguously. (See eg Gasiorowicz and Geffen (1969) for a review of this and other relevant material.)

In most applications the Lagrange density (1.1) has been used only to lowest contributing order in a perturbation expansion. This means that only tree-graph diagrams contributing to the process under consideration are evaluated. Thus no divergences are encountered since there are no loop momenta over which integrations would have to be performed, and the problems associated with the nonrenormalizability of (1.1) are avoided. Attempts have been made to discuss the inclusion of closed loops (see eg

Charap (1970, 1971) and references in this latter paper, especially Gerstein *et al* (1971)), and the pion superpropagator has been determined (Davies 1972). However, in these discussions attention has not been paid to the need to consider the order of noncommuting factors which appear in (1.1). The problems of ordering have been discussed elsewhere, and we shall return to the work of other authors in the concluding section of this paper. What we want to do in this paper is to consider the question of the order of factors if (1.1) is to be taken as the basis for a *quantum* field theory with chiral invariance.

This problem of the order of factors is already present in quantum mechanics, and since the extra problems associated with field theory might only serve to obscure the main issue, we discuss a system with a finite number of degrees of freedom for which the classical Lagrangian, analogous to (1.1) is

$$L = \tfrac{1}{2}\dot{q}^i g_{ij}(q)\dot{q}^j. \tag{1.4}$$

This classical system is outlined in § 2. Using what are in essence the methods advocated by Dirac, we show in § 3 how to quantize the system in the canonical way. At this stage we retain the ambiguities associated with re-ordering noncommuting factors. In this same section we also emphasize that one should not construct a quantum operator analogue for (1.4) from which the equations of motion might be derived as Euler–Lagrange equations. We show that it is not possible in any but trivial cases for this to be done in such a way that the Euler–Lagrange equations of motion are consistent with the Hamilton equations, or Heisenberg equations as they are in the quantum-mechanical formulation.

For this reason we prefer to discuss the imposition of a symmetry on the theory in the canonical, Hamiltonian formulation, rather than with the Lagrangian, as is perhaps more familiar. Section 4 is concerned with the imposition of chiral invariance. There are of course ambiguities associated with the construction of operators V^i and A^j which generate the algebra and which have an action on the variables q^k analogous to (1.2) and (1.3). These ambiguities are associated with trivial unitary transformations of the representation of the algebra, but once the group generators are constructed the Hamiltonian, if it is to be invariant, is *uniquely* determined, with the ambiguities associated with factor ordering completely removed. The result is in fact just a constant multiple of the quadratic Casimir operator. This 'charge–charge' form for the Hamiltonian is highly reminiscent of the 'current–current' form of the energy–momentum tensor in the model of chiral invariant field theory proposed by Sugawara (1968). We conclude § 4 with a brief discussion of the Schrödinger representation of our model. Finally, in § 5, we discuss our result and compare it with the work of other authors.

2. A classical system

Consider first a classical system with generalized coordinates $q^i (i = 1, 2, \ldots, n)$, and corresponding velocities $\dot{q}^i$. Suppose that the Lagrangian for the system is of the form

$$L = \tfrac{1}{2}g_{ij}\dot{q}^i\dot{q}^j \tag{2.1}$$

where the g_{ij} are as yet unspecified functions of the coordinates q. We may without loss of generality suppose that the matrix $\|g_{ij}\|$ is, however, symmetrical. Canonically conjugate to the coordinate q^i is the momentum p_i, defined as usual by

$$p_i \equiv \frac{\partial L}{\partial \dot{q}^i} = g_{ij}\dot{q}^j. \tag{2.2}$$

We henceforth suppose that the matrix $\|g_{ij}\|$ is nonsingular, and write its inverse as $\|g^{ij}\|$. Then (2.2) may be inverted to give the velocities in terms of the momenta,

$$\dot{q}^i = g^{ij}p_j. \tag{2.3}$$

Following standard procedure, the Hamiltonian is obtained by making the Legendre transform

$$H(q,p) \equiv p_i\dot{q}^i - L = \tfrac{1}{2}g^{ij}p_ip_j. \tag{2.4}$$

Hamilton's equations of motion are $\dot{q}^i = \partial H/\partial p_i$, which just recover (2.3), and

$$\dot{p}_i = \frac{-\partial H}{\partial q^i} = -\tfrac{1}{2}g^{jk}{}_{,i}p_jp_k. \tag{2.5}$$

The notation introduced here is to write $\partial A/\partial q^i$ as $A_{,i}$. From (2.5) together with (2.2) we obtain

$$g_{ij}\ddot{q}^j + \dot{g}_{ij}\dot{q}^j = -\tfrac{1}{2}g^{jk}{}_{,i}g_{jl}\dot{q}^l g_{km}\dot{q}^m$$

or on applying the identity

$$g^{jk}{}_{,i}g_{km} + g^{jk}g_{km,i} \equiv 0 \tag{2.6}$$

we may recover Lagrange's equations of motion, which are

$$\ddot{q}^j + \Gamma^j_{kl}\dot{q}^k\dot{q}^l = 0. \tag{2.7}$$

The Christoffel symbol Γ^j_{kl} is defined by

$$\Gamma^j_{kl} \equiv \tfrac{1}{2}g^{ij}(g_{ik,l} + g_{il,k} - g_{kl,i}). \tag{2.8}$$

If the coordinates q are regarded as coordinates of a point in a riemannian manifold $\mathcal{M}_n$ with metric tensor $g_{ij}(q)$, the equation of motion (2.7) shows that the motion takes place along geodesics of $\mathcal{M}_n$. This was in any case to be expected since the Lagrangian (2.1) may also be written as

$$L = \frac{1}{2}g_{ij}\frac{dq^i dq^j}{(dt)^2} = \frac{1}{2}\left(\frac{ds}{dt}\right)^2$$

where

$$ds^2 \equiv g_{ij}dq^i dq^j \tag{2.9}$$

is the metric of $\mathcal{M}_n$.

3. The quantum-mechanical analogue

If we wish to construct a quantum-mechanical analogue to the classical system described in the previous section, it is permissible to start by writing down the canonical commutation relations

$$[q^i, p_j] = \mathrm{i}\delta^i_j \tag{3.1}$$

$$[q^i, q^j] = 0 \tag{3.2}$$

$$[p_i, p_j] = 0. \tag{3.3}$$

To specify the dynamics we must choose a hamiltonian operator which is of the same form as in the classical case (equation (2.4)); but we are now required to specify an order in which the factors are to be written. The most general form is equivalent to taking

$$H = \tfrac{1}{8}\{p_i, \{p_j, g^{ij}\}\} + \tfrac{1}{2}\{p_i, u^i\} + v. \tag{3.4}$$

We have used the notation $\{A, B\}$ to denote the anticommutator of two operators, $\{A, B\} \equiv AB + BA$, and have introduced u^i and v, arbitrary functions of the coordinate operator q. If these functions tend to zero with the Planck constant, and if the matrix $\|g^{ij}\|$ is the same function of the operators q as was the matrix $\|g^{ij}\|$ of the coordinates q in the classical case, it is clear that H as defined in (3.4) is a suitable quantum Hamiltonian analogous to (2.4). Furthermore if u^i and v are real functions, H is hermitian.

The Heisenberg form of the equations of motion give

$$\begin{aligned} \dot{q}^i &= \mathrm{i}[H, q^i] \\ &= \tfrac{1}{2}\{g^{ik}, p_k\} + u^i \end{aligned} \tag{3.5}$$

and for any function $G(q)$,

$$\dot{G} = \tfrac{1}{2}\{G_{,k}, \dot{q}^k\}. \tag{3.6}$$

We also have

$$\begin{aligned} \dot{p}_i &= \mathrm{i}[H, p_i] \\ &= -\tfrac{1}{8}\{p_l, \{p_m, g^{lm}_{,i}\}\} - \tfrac{1}{2}\{p_l, u^l_{,i}\} - v_{,i}. \end{aligned} \tag{3.7}$$

Equation (3.5) may be inverted to obtain

$$p_i = \tfrac{1}{2}\{g_{ik}, \dot{q}^k\} - u_i \tag{3.8}$$

where we have introduced u_i defined by

$$u_i \equiv g_{ij}u^j. \tag{3.9}$$

The problem we wish now to consider relates to the Lagrangian. There is a certain amount of confusion about the role of the Lagrangian in quantum mechanics. We do not wish to make any comment about the Feynman method of quantization in which the Lagrangian appears as a c number, and the subtleties of ordering noncommuting factors are translated into subtleties of definition of functional integrals. In the more conventional methods of passage from a classical to a quantum-mechanical description of a system, it is a canonical formulation which is used, in which coordinates and momenta are the dynamical variables, and velocities are given a meaning only through the equations of motion. Nonetheless, especially in formulating relativistic quantum field theories, it often happens that an expression in terms of coordinates and velocities (or fields and their gradients) is described as a Lagrangian, and equations of motion derived as Euler–Lagrange equations, even though the formulation is supposed to be quantum mechanical, not classical.

What we want to criticize then is this use of an *operator* function L of coordinates and velocities, treated as though one can proceed as in classical mechanics to derive the equations

$$\frac{\partial L}{\partial \dot{q}^i} = p_i \tag{3.10}$$

and (Lagrange's equations)

$$\frac{\partial L}{\partial q^i} = \dot{p}_i. \tag{3.11}$$

The difficulty lies in giving a meaning to the partial differentials with respect to q numbers on the left hand sides of these equations. The correct and conventional approach is to find some way to replace the partial differentials by commutators. Clearly this is not going to be easy, for although we have

$$[q^i, q^j] = 0 \tag{3.2}$$

using (3.5) we obtain

$$[q^i, \dot{q}^j] = \mathrm{i}g^{ij} \tag{3.12}$$

and

$$[\dot{q}^i, \dot{q}^j] = \tfrac{1}{2}\mathrm{i}\{\dot{q}^k, (g^{il}g^{jm} - g^{jl}g^{im})g_{km,l}\} - \mathrm{i}(g^{il}u^j_{,l} - g^{jl}u^i_{,l}). \tag{3.13}$$

What is certainly true is that any definition of the partial differentiation must obey the usual rules for differentiation (in particular Leibniz' rule for products) and will respect the order of q number factors.

To satisfy (3.10), the Lagrangian must be quadratic in the velocities, so we may write

$$L = \tfrac{1}{8}\{\dot{q}^k, \{\dot{q}^l, \hat{g}_{kl}\}\} - \tfrac{1}{2}\{\dot{q}^k, \hat{u}_k\} - w. \tag{3.14}$$

Consistency of (3.8) and (3.10) then implies the unsurprising identifications

$$\hat{g}_{kl} = g_{kl} \tag{3.15}$$

and

$$\hat{u}_k = u_k. \tag{3.16}$$

On the other hand to make (3.11) consistent with (3.7) we require in addition

$$4(v - w - \tfrac{1}{2}u^k u_k)_{,i} + g^{kr}_{,i}(g_{kl}g^{ls}_{,s})_{,r} = 0. \tag{3.17}$$

These equations may be treated as equations for the determination of w, but being partial differential equations they are not even self-consistent unless appropriate integrability conditions are satisfied. These conditions,

$$g^{kr}_{,i}(g_{kl}g^{ls}_{,s})_{,rj} = g^{kr}_{,j}(g_{kl}g^{ls}_{,s})_{,ri} \tag{3.18}$$

are by no means trivial. Indeed for most cases of interest, and certainly in general, they are *not* satisfied. This means that in general there is *no* choice of Lagrangian for which the Lagrange equations of motion (as we have interpreted them) are consistent with the canonical Hamilton–Heisenberg equations.

As we have indicated, the difficulty is associated with the appearance on the right hand sides of (3.12) and (3.13) of q numbers. To see more clearly how this leads to the root of the problem, we recognize that what we are seeking are two sets of operators A_i and B_i so defined as to make acceptable the replacements

$$\frac{\partial F(q,\dot{q})}{\partial q^i} \rightarrow \mathrm{i}[F, A_i]$$

$$\frac{\partial F(q,\dot{q})}{\partial \dot{q}^i} \rightarrow \mathrm{i}[F, B_i].$$

Evidently these require

$$\mathrm{i}[q^j, A_i] = \delta_i^j$$

$$\mathrm{i}[\dot{q}^j, A_i] = 0;$$

and

$$\mathrm{i}[q^j, B_i] = 0$$

$$\mathrm{i}[\dot{q}^j, B_i] = \delta_i^j.$$

It is the first of these pairs of equations which is the principal stumbling block. For a consideration of the Jacobi identity for the double commutators of A_i, q^j and $\dot{q}^k$ shows there to be no solution unless the matrix $\|g_{ij}\|$ is constant.

The second pair of equations can be solved in the special case when the velocities commute. This situation is not of interest for problems like those of chiral dynamics.

We conclude that there really is no way to give a satisfactory meaning to the Lagrange equations of motion in the quantum-mechanical treatment unless $\|g_{ij}\|$ is constant, and of course in that case (3.17) becomes

$$v - w - \tfrac{1}{2}u^k u_k = \text{constant}; \tag{3.18}$$

the constant may without loss of generality be set equal to zero.

Since in any case from (3.4) and (3.13) we have

$$H + L = \tfrac{1}{2}\{p_i, \dot{q}^i\} + (v - w - \tfrac{1}{2}u^k u_k) \tag{3.19}$$

we learn that the Lagrangian and the Hamiltonian are, in the case of constant g_{ij}, connected by the Legendre transform

$$L = \tfrac{1}{2}\{p_i, \dot{q}^i\} - H.$$

The case of constant $\|g_{ij}\|$ is not of any interest however. For noting that $\|g_{ij}\|$ is a positive-definite matrix, it has a real matrix square root $\|r_{ij}\|$. The change of variables from q to Q given by

$$Q^i = \delta^{ik} r_{kl} q^l$$

then reduces the original classical Lagrangian to the Lagrangian

$$L = \tfrac{1}{2}\dot{Q}^i \delta_{ij} \dot{Q}^j \tag{3.20}$$

of a free system.

4. Symmetry

In this section we wish to explore the consequences for the expressions g^{ij}, u^i and v which enter into the equation (3.4) for the Hamiltonian if the system possesses a group

G of symmetries generated by some Lie algebra. Suppose therefore that there are a set F^a, $a = 1, 2, \ldots, N$, of operators with the commutation relations

$$[F^a, F^b] = \mathrm{i}f^{ab}{}_cF^c; \tag{4.1}$$

the c numbers $f^{ab}{}_c$ are the structure constants of the algebra. Suppose further that the action of the group is pointwise on the manifold $\mathscr{M}_n$ with coordinates q^i, so that

$$[F^a, q^i] = \mathrm{i}f^{ai}(q) \tag{4.2}$$

for some functions f^{ai}. The group structure, as embodied in the Jacobi identity for the double commutators of F^a, F^b and q^i, leads to

$$f^{aj}f^{bi}{}_{,j} - f^{bj}f^{ai}{}_{,j} = f^{ab}{}_cf^{ci}. \tag{4.3}$$

We must determine the action of the group on the momenta p_i. If we suppose the action of G to be linear in the momenta, then for some functions $h^{aj}{}_i(q)$ and $h^a{}_i(q)$, we have

$$[F^a, p_i] = -\tfrac{1}{2}\mathrm{i}\{h^{aj}{}_i, p_j\} + \mathrm{i}h^a{}_i. \tag{4.4}$$

The Jacobi identity on the double commutators of F^a, p_i and q^j implies

$$h^{aj}{}_i = f^{aj}{}_{,i} \tag{4.5}$$

whilst that on F^a, p_i and p_j implies

$$h^a_{i,j} = h^a_{j,i}. \tag{4.6}$$

From this it follows that there exist functions $h^a(q)$ for which

$$h^a{}_i = h^a{}_{,i}. \tag{4.7}$$

The Jacobi identity for F^a, F^b and p_i then implies

$$f^{ai}h^b_{,i} - f^{bi}h^a_{,i} = f^{ab}{}_ch^c \tag{4.8}$$

which is equivalent to the group law

$$[F^a, h^b] - [F^b, h^a] = \mathrm{i}f^{ab}{}_ch^c. \tag{4.9}$$

We note that if h is any dynamical variable, then an application of the Jacobi identity shows directly that h^a, given by

$$h^a = -\mathrm{i}[F^a, h] \tag{4.10}$$

is a solution to (4.8) or (4.9).

From (4.2) and the equation obtained from (4.4), namely

$$[F^a, p_i] = -\tfrac{1}{2}\mathrm{i}\{f^{aj}{}_{,i}, p_j\} + \mathrm{i}h^a{}_{,i} \tag{4.11}$$

it follows that the generators may be expressed as

$$F^a = -\tfrac{1}{2}\{f^{ai}, p_i\} + h^a. \tag{4.12}$$

We are now in a position to evaluate $[F^a, H]$ using (3.4). The result is

$$[F^a, H] = -\tfrac{1}{8}\mathrm{i}\{p_i, \{p_j, K^{aij}\}\} - \tfrac{1}{2}\mathrm{i}\{p_i, K^{ai}\} - \mathrm{i}K^a \tag{4.13}$$

where the various functions K of q are given by

$$K^{aij} = f^{aj}{}_{,k}g^{ik} + f^{ai}{}_{,k}g^{jk} - f^{ak}g^{ij}{}_{,k} \tag{4.14}$$

$$K^{ai} = f^{ai}{}_{,j}u^{j} - f^{aj}u^{i}{}_{,j} - g^{ij}h^{a}{}_{,j} \tag{4.15}$$

and

$$K^{a} = \tfrac{1}{8}f^{ak}{}_{,ij}g^{ij}{}_{,k} - f^{ai}v_{,i} - h^{a}{}_{,i}u^{i}. \tag{4.16}$$

The condition for the group G generated by the F^a to be a symmetry is

$$[F^a, H] = 0 \tag{4.17}$$

which means then that all the functions K must vanish.

The conditions imposed by the vanishing of K^{aij} are already applicable in classical theory. They are none other than Killing's equations for g_{ij} which are the conditions that $g_{ij}\,\mathrm{d}q^i\,\mathrm{d}q^j$ shall be a group-invariant metric on $\mathscr{M}_n$. One situation which might arise is when the action on $\mathscr{M}_n$ is linear. Killing's equations then imply that g^{ij} is a second rank tensor of the group. This is not the situation we wish to consider, rather let us suppose the action of G to be nonlinear. There is still a solution to Killing's equations, namely

$$g^{ij} = \nu e_{ab} f^{ai} f^{bj} \tag{4.18}$$

where ν is an arbitrary constant (which may be chosen so that $g^{ij} = \delta^{ij}$ for $q = 0$) and e_{ab} is the matrix inverse to e^{ab}, which is in turn given by

$$e^{ab} = f^{ac}{}_{d} f^{db}{}_{c}. \tag{4.19}$$

For the situation of principal physical interest, to which we henceforth confine ourselves, G will be a chiral group; $G = \mathrm{SU}(m)_\mathrm{L} \times \mathrm{SU}(m)_\mathrm{R}$. The suffices L and R distinguish between the 'left hand' and 'right hand' subgroups, which are interchanged by the parity operation which is an external automorphism of G. The case of physical interest is then obtained by asking that the parity-conserving 'diagonal' subgroup $\mathrm{SU}(m)$ of G shall act linearly on G. The coordinates q^i ($i = 1, 2, \ldots, n = m^2-1$) transform under the adjoint representation of this diagonal subgroup. If the generators F^a are separated into the two sets F^i_+ and F^i_-, generators of the commuting $\mathrm{SU}(m)_\mathrm{R}$ and $\mathrm{SU}(m)_\mathrm{L}$ respectively, ($N = 2(m^2-1)$), then, with a corresponding notation we have

$$f^{ij}_{\pm} = f^{ij}(q) \pm f^{ij}{}_{k}q^{k} \tag{4.20}$$

where the matrix f^{ij} is a symmetrical second rank tensor of the diagonal subgroup and is an even function of q. The constants $f^{ij}{}_k$ are the structure constants of the diagonal subgroup. The matrices $f^{ij}_{\pm}$ are nonsingular. We also note that (4.18) may be replaced by

$$g^{ij} = \nu'\delta_{kl} f^{ki}_{+} f^{lj}_{+} = \nu'\delta_{kl} f^{ki}_{-} f^{lj}_{-}; \tag{4.21}$$

again ν' is a normalization constant.

We turn next to the equations consequent upon the vanishing of K^{ai}. Let us define $k^j_{\pm}$ by

$$k^j_{\pm} \equiv f^{ji}_{\pm} u_i. \tag{4.22}$$

Then using (4.21) we have

$$\nu'\delta_{kl} f^{kj}_{\pm} k^l_{\pm} = u^j \tag{4.23}$$

so that the vanishing of K^{ai},

$$g^{ij}h^a{}_{,j} = f^{ai}{}_{,j}u^j - f^{aj}u^i{}_{,j}$$

is equivalent to

$$g^{ij}h^a{}_{,j} = v'\delta_{kl}[(f^{ai}{}_{,j}f^{kj}_{\pm} - f^{aj}f^{ki}_{\pm,j})k^l_{\pm} - f^{aj}f^{ki}_{\pm}k^l_{\pm,j}].$$

Using (4.3) this leads to

$$g^{ij}h^m_{\pm,j} = -v'\delta_{kl}f^{ki}_{\pm}(f^{lm}{}_n k^n_{\pm} + f^{mj}_{\pm}k^l_{\pm,j})$$

and

$$g^{ij}h^m_{\mp,j} = -v'\delta_{kl}f^{mj}_{\mp}f^{ki}_{\pm}k^l_{\pm,j}.$$

Using (4.21) and the invertibility of $\| f^{ki}_{\pm}\|$, we obtain

$$f^{lj}_{\pm}h^m_{\pm,j} = -(f^{lm}{}_n k^n_{\pm} + f^{mj}_{\pm}k^l_{\pm,j})$$

and

$$f^{lj}_{\pm}h^m_{\mp,j} = -f^{mj}_{\mp}k^l_{\pm,j}.$$

Then from (4.8), we conclude

$$f^{mj}_{\pm}(k^l_{\pm} + h^l_{\pm})_{,j} = f^{ml}{}_n(k^n_{\pm} + h^n_{\pm})$$

and

$$f^{mj}_{\mp}(k^l_{\pm} + h^l_{\pm})_{,j} = 0.$$

The invertibility of the matrices $\| f^{mj}_{\pm}\|$ then allows directly the conclusion

$$k^l_{\pm} + h^l_{\pm} = 0 \tag{4.24}$$

so that, using (4.23),

$$u^j = -v'\delta_{kl}f^{kj}_{\pm}h^l_{\pm}. \tag{4.25}$$

Finally we consider the consequences of the vanishing of the quantities K^a defined in (4.16). To facilitate this, let us prove first

$$f^{ai}{}_{,jk}g^{jk}{}_{,i} = ve_{bc}(f^{bi}{}_{,j}f^{cj}{}_{,i})_{,k}f^{ak}. \tag{4.26}$$

For we have

$$\begin{aligned}
&ve_{bc}(f^{bi}{}_{,j}f^{cj}{}_{,i})_{,k}f^{ak} - f^{ai}{}_{,jk}g^{jk}{}_{,i}\\
&\qquad = 2ve_{bc}(f^{bi}{}_{,jk}f^{cj}{}_{,i}f^{ak} - f^{ai}{}_{,jk}f^{cj}{}_{,i}f^{bk})\\
&\qquad = 2ve_{bc}f^{cj}{}_{,i}[(f^{bi}{}_{,k}f^{ak} - f^{ai}{}_{,k}f^{bk})_{,j} - f^{bi}{}_{,k}f^{ak}{}_{,j} + f^{ai}{}_{,k}f^{bk}{}_{,j}]\\
&\qquad = 2ve_{bc}f^{cj}{}_{,i}(f^{ab}{}_d f^{di}{}_{,j} - f^{bi}{}_{,k}f^{ak}{}_{,j} + f^{ai}{}_{,k}f^{bk}{}_{,j})\\
&\qquad = 2ve_{bc}f^{ab}{}_d f^{cj}{}_{,i}f^{di}{}_{,j} - 2ve_{bc}f^{ak}{}_{,j}(f^{bi}{}_{,k}f^{cj}{}_{,i} - f^{bj}{}_{,i}f^{ci}{}_{,k})\\
&\qquad = 0.
\end{aligned}$$

In the steps of the proof we have used successively (4.18), (4.3), a rearrangement of dummy indices, and the fact that $e_{bc}f^{ab}{}_d$ is antisymmetrical in c, d whilst e_{bc} is symmetrical in b, c. It now follows that

$$K^a = (\tfrac{1}{8}ve_{bc}f^{bc}{}_{,j}f^{cj}{}_{,i} - v)_{,k}f^{ak} - h^a{}_{,k}u^k$$

but using

$$u^j = -ve_{ab}f^{bj}h^a \tag{4.27}$$

which is an immediate consequence of (4.25), and also (4.8), we have

$$\begin{aligned} h^a{}_{,k}u^k &= -h^a{}_{,k}ve_{bc}f^{bk}h^c \\ &= -ve_{bc}h^c(h^b{}_{,k}f^{ak}+f^{ba}{}_d h^d) \\ &= -(\tfrac{1}{2}ve_{bc}h^bh^c)_{,k}f^{ak}. \end{aligned} \tag{4.28}$$

So we may write

$$K^a = (\tfrac{1}{8}ve_{bc}f^{bi}{}_{,j}f^{cj}{}_{,i} - v + \tfrac{1}{2}ve_{bc}h^bh^c)_{,k}f^{ak}. \tag{4.29}$$

The vanishing of K^a, together with the invertibility of the matrices $\|f^{mk}_{\pm}\|$ thus leads to

$$v = \tfrac{1}{2}ve_{bc}(h^bh^c + \tfrac{1}{4}f^{bi}{}_{ij}f^{cj}{}_{,i}) \tag{4.30}$$

where we have dropped an arbitrary additive constant.

Before going further, let us collect together the principal equations we wish to work with. They are

$$H = \tfrac{1}{8}\{p_i, \{p_j, g^{ij}\}\} + \tfrac{1}{2}\{p_i, u^i\} + v \tag{3.4}$$

$$F^a = -\tfrac{1}{2}\{f^{ai}, p_i\} + h^a \tag{4.12}$$

$$g^{ij} = ve_{ab}f^{ai}f^{bj} \tag{4.18}$$

$$u^j = -ve_{ab}h^af^{bj} \tag{4.27}$$

and the expression (4.30) for v above. It follows directly that we always have

$$H = \tfrac{1}{2}ve_{ab}F^aF^b. \tag{4.31}$$

All the operators in these equations are hermitian. Since ve_{ab} is positive definite, it follows that H is, as it should be, a positive semi-definite operator.

It will be seen that the only ambiguity in the expression (4.31) for the group-invariant Hamiltonian, given the transformation law (4.2) for the coordinates, is in the functions h^a. In (4.10) we gave a form of solution for these functions. We now show that this form is general. For if we define h_i by

$$h_i = vg_{ij}f^{aj}h^be_{ab}, \tag{4.32}$$

for any functions $h^b(q)$ satisfying (4.9), it is straightforward to show that

$$h_i = h_{,i} \tag{4.33}$$

for some function $h(q)$; and then

$$\begin{aligned} h^a &= f^{ai}h_{,i} \\ &= -\mathrm{i}[F^a, h]. \end{aligned} \tag{4.34}$$

But if we take $\hat{F}^a$ so that

$$\hat{F}^a = -\tfrac{1}{2}\{f^{ai}, p_i\}$$

then it is also true that

$$h^a = -\mathrm{i}[\hat{F}^a, h]$$

and it follows directly that we have

$$\begin{aligned} F^a &= \hat{F}^a + h^a \\ &= \exp(\mathrm{i}h)\hat{F}^a \exp(-\mathrm{i}h). \end{aligned} \tag{4.35}$$

Thus we see that changing the functions h^a in (4.12) is accomplished by a unitary transformation on the solutions F^a of (4.1) and of H given through (4.31). To within a unitary equivalence the group-invariant Hamiltonian is unique.

Should we wish to set up a representation for the operators on a Hilbert space of functions of q, that is, of functions on $\mathscr{M}_n$, we must take a further step. The states are represented by wavefunctions $\psi(q)$, and of course the operators representing the coordinates q^i are just multiplicative. This does not yet specify the form taken by the momentum operators p_i, because the commutation relations,

$$[q^i, p_j] = \mathrm{i}\delta^i_j \tag{3.1}$$

$$[p_i, p_j] = 0 \tag{3.3}$$

have as solution

$$p_j = -\frac{\mathrm{i}\partial}{\partial q_j} - \mathrm{i}\Gamma_{,j} \tag{4.36}$$

where Γ is any function of the coordinates q. To determine Γ it is necessary to specify how scalar products are to be taken in the Hilbert space. Let us write

$$\langle\phi|\psi\rangle = \int \phi^*(q)\psi(q)w(q)\,\mathrm{d}^n q \tag{4.37}$$

where the integration is over the whole of the coordinate space and $w(q)$ is a real non-negative weight function. Then the requirement that p_j as given by (4.36) shall be hermitian relates Γ and w through

$$\Gamma = \ln\sqrt{w}. \tag{4.38}$$

Corresponding to (4.36) we have

$$\begin{aligned} \hat{F}^a &= \tfrac{1}{2}\mathrm{i}\{f^{ai}, \partial_i\} + \mathrm{i}f^{ai}\Gamma_{,i} \\ &= \tfrac{1}{2}\mathrm{i}\{f^{ai}, \partial_i\} + [\hat{F}^a, \Gamma]. \end{aligned} \tag{4.39}$$

We have written ∂_i for the differential operator $\partial/\partial q^i$. The second term cannot be eliminated by a unitary transformation of course, since Γ is a real function of q.

If we ask that the scalar products in the Hilbert space shall be specified in a group-invariant fashion, then $w(q)\mathrm{d}^n q$ must be the group-invariant measure on $\mathscr{M}_n$. This means that to within a constant factor we have

$$w(q) = \sqrt{g} \tag{4.40}$$

where we have introduced g, defined as usual by

$$g \equiv \det\|g_{ij}\|. \tag{4.41}$$

Then (4.36) becomes

$$p_i = -\mathrm{i}\partial_i - \tfrac{1}{4}\mathrm{i}(\ln g)_{,i} \tag{4.42}$$

and (4.40) reads

$$\hat{F}^a = \mathrm{i}\tfrac{1}{2}\{f^{ai}, \partial_i\} + \mathrm{i}\tfrac{1}{4}f^{ai}(\ln g)_{,i}. \tag{4.43}$$

It is always true for any symmetric matrix $\|g_{ij}\|$ that

$$(\ln g)_{,i} = g^{jk}g_{jk,i}$$

and since Killing's equations imply

$$f^{ai}g_{jk,i} = -f^{ai}{}_{,j}g_{ik} - f^{ai}{}_{,k}g_{ij}$$

we obtain

$$f^{ai}(\ln g)_{,i} = -2f^{ai}{}_{,i}. \tag{4.44}$$

Hence we have

$$\hat{F}^a = \mathrm{i}\tfrac{1}{2}\{f^{ai}, \partial_i\} - \mathrm{i}\tfrac{1}{2}f^{ai}{}_{,i} \tag{4.45}$$

$$= \mathrm{i}f^{ai}\partial_i = \mathrm{i}g^{-1/2}\partial_i g^{1/2}f^{ai}. \tag{4.46}$$

For the Hamiltonian this gives

$$\begin{aligned} H &= \tfrac{1}{2}ve_{ab}\hat{F}^a\hat{F}^b \\ &= -\tfrac{1}{2}ve_{ab}f^{ai}\partial_i f^{bj}\partial_j \\ &= -\tfrac{1}{2}g^{-1/2}\partial_i g^{1/2}g^{ij}\partial_j \\ &\equiv -\tfrac{1}{2}\Delta_2. \end{aligned} \tag{4.47}$$

Here Δ_2 is the Laplace–Beltrami operator on the curved manifold $\mathcal{M}_n$.

The Schrödinger equation of motion for the wavefunction $\psi(q, t)$, normalized so that

$$\langle\psi|\psi\rangle \equiv \int |\psi(q, t)|^2 g^{1/2}(q)\,\mathrm{d}q = 1 \tag{4.48}$$

is

$$\mathrm{i}D_t\psi = H\psi = -\tfrac{1}{2}\Delta_2\psi. \tag{4.49}$$

Here D_t denotes the conservative time derivative,

$$D_t\psi \equiv g^{-1/4}\frac{\partial}{\partial t}(g^{1/4}\psi) \tag{4.50}$$

which is appropriate to the normalization (4.48) above. In other words, just as coordinate displacements are given by (cf (4.42))

$$\partial_i = \mathrm{i}g^{1/4}p_i g^{-1/4}, \tag{4.51}$$

so, also, time displacements are given by

$$\frac{\partial}{\partial t} = -\mathrm{i}g^{1/4}Hg^{-1/4}. \tag{4.52}$$

If we define the reduced wavefunction $\hat{\psi}$ by

$$\hat{\psi} = g^{1/4}\psi, \tag{4.53}$$

we have the normalization

$$\langle\psi|\psi\rangle = \int |\hat{\psi}|^2 \, \mathrm{d}q = 1 \tag{4.54}$$

the matrix elements

$$\begin{aligned} \langle\phi|q^i|\psi\rangle &= \int \phi^* q^i \psi g^{1/2} \, \mathrm{d}q \\ &= \int \hat{\phi}^* q^i \hat{\psi} \, \mathrm{d}q \end{aligned} \tag{4.55}$$

$$\begin{aligned} \langle\phi|p_i|\psi\rangle &= -\mathrm{i} \int \phi^* g^{-1/4} \partial_i (g^{1/4}\psi) g^{1/2} \, \mathrm{d}q \\ &= -\mathrm{i} \int \hat{\phi}^* \partial_i \hat{\psi} \, \mathrm{d}q \end{aligned} \tag{4.56}$$

and the Schrödinger equation

$$\begin{aligned} \frac{\mathrm{i}\partial}{\partial t}\hat{\psi} &= (g^{1/4} H g^{-1/4})\hat{\psi} \\ &= -\tfrac{1}{2} g^{1/4} \Delta_2 g^{-1/4} \hat{\psi}. \end{aligned} \tag{4.57}$$

Finally we record the forms

$$H = \tfrac{1}{2} p_i g^{ij} p_j - \tfrac{1}{2} g^{1/4} \Delta_2 g^{-1/4} = \tfrac{1}{2} g^{-1/4} p_i g^{ij} g^{1/2} p_j g^{-1/4}. \tag{4.58}$$

5. Discussion

Many of the topics considered in this paper have been treated earlier by other authors. The problem of ordering noncommuting factors is of course almost as old as quantum mechanics but the first treatment in the spirit of the present paper seems to be by DeWitt (1952). In that paper he argues that invariance under an appropriate group of point transformations is indeed the criterion which should be adopted in order to resolve questions of factor ordering. He considers the Lagrangian (1.4), and its generalization (3.14), and makes the sweeping claim that such Lagrangians 'include all systems in nature which satisfy Bose–Einstein statistics'. This claim is repeated in a later paper (DeWitt 1957) which continues his treatment of quantum mechanics on curved spaces. The emphasis in this paper is on action principles, with which we have not been concerned in the present work.

The breakdown of the usual connection between Lagrangian and Hamiltonian through the Legendre transform (2.4) for the quantum-mechanical case has been pursued by Sugano and his co-workers (Kiang *et al* 1969, Lin *et al* 1970, Sugano 1971, Kimura 1971, Kimura and Sugano 1972, Ohtani and Sugano 1972). Again they consider systems for which the classical Lagrangian is of the form (1.4). They show that when the space for which g_{ij} is the metric tensor is flat ($R^i{}_{jkl} = 0$), there exists a point transformation which brings the Lagrangian to the form (3.20). It should be noted that we used constant g_{ij} to obtain (3.20), a stronger requirement, but in any case we are agreed that the main interest is in curved, not flat, manifolds. In the most recent of the works cited (Ohtani and Sugano 1972) consideration was extended to curved manifolds, but only to spaces of constant ourvature (Einstein spaces). This is indeed adequate for the problem of chiral invariant models, for as is well known, the relevant manifolds, even for $\mathrm{SU}(n) \times \mathrm{SU}(n)$ are Einstein spaces. They obtain as their Hamiltonian an expression which differs from (4.47) only by an arbitrary function of the curvature scalar R; but, since in any case R is a c number, this makes no difference to the dynamics. They show that the Lagrangian

$$L = \tfrac{1}{8} g^{-1/4}\{g_{ik}\dot{q}^k\} g^{1/2} g^{ij} \{g_{jl}\dot{q}^l\} g^{-1/4}$$

does yield the same equations of motion as the Hamilton–Heisenberg equations, but only with a variational principle which differs from the usual one in that the variations are restricted so that

$$\delta\dot{q}^i = \frac{\mathrm{d}\delta q^i}{\mathrm{d}t}.$$

The form of the Hamiltonian derived by Ohtani and Sugano was already given by DeWitt (1957). He gives some discussion of the extra term involving R (this term can, on dimensional grounds, only be a constant multiple of $\hbar^2 R$); of course when the manifold is not of constant curvature, this discussion has physical relevance. This point is taken up and pursued further by Dowker and Mayes (1971). The main object of their paper, however, is directed to canonical quantization. They start with the Schrödinger equation, but overlook the need when using the normalization (4.48) to use the conservative time derivative; this point is explained by DeWitt (1957). However, since they proceed correctly to derive the hamiltonian operator in a form equivalent to (4.58), this oversight is not crucial. Their choice of Schrödinger equation, and in particular the use of the Laplace–Beltrami operator, was made because they wanted chiral-invariant dynamics. The exclusion of terms involving R, $R_{ij}R^{ij}$, etc was justified 'by a sort of minimal principle'; but as they all but state explicitly, such terms are constants for the chiral case.

They then go on to obtain an expression for the Feynman propagator, namely

$$\langle q'', t'' | q', t' \rangle = \mathcal{N} \int \mathscr{D}(q) \exp\left(\mathrm{i} \int_{t'}^{t''} \mathrm{d}t (L - B) \right).$$

In this expression $\mathcal{N}$ is just a normalization constant, and $\mathscr{D}(q)$ is a functional measure on the paths in the manifold, related to the cartesian measure $d(q)$ through

$$\mathscr{D}(q) = \exp\left(\tfrac{1}{2}\delta(0) \int \ln g \,\mathrm{d}t \right) d(q).$$

This is a necessary modification which escaped the present author in a different context (Charap 1970), but has received a deal of attention elsewhere (eg Charap (1971), the earliest reference I can trace is Lee and Yang (1962), although the result is already implicit in DeWitt (1957)).

More relevant to the present discussion is the term B. This term arises in giving a meaning to the functional integrals which appear in the canonical expression for the propagator, namely

$$\langle q'', t''|q', t'\rangle = \mathcal{N}\int d(p)\int d(q)\exp(\mathrm{i}A),$$

with

$$A = \int_{t'q'}^{t''q''} (p\,\mathrm{d}q - H_\mathrm{c}(pq)\,\mathrm{d}t).$$

This is discussed by the same authors (Mayes and Dowker 1972, 1973). The point is that, given a classical Hamiltonian H_c, different definitions of the functional integrals lead to different corresponding quantum Hamiltonians. The argument may be inverted, since we have an explicit form for the quantum Hamiltonian (viz (4.58)), and we are then led to ask: given a method of defining the functional integrals, what should be used as the classical Hamiltonian H_c? Their conclusion is that for *no* choice of definition of the functional integral may H_c be identified with (2.4). There is always to be added an extra term, and this is just the term B. To be explicit, with the so-called symmetrization rule for defining the functional integrals, they obtain

$$B = \tfrac{1}{4}g^{ij}_{,ij} - \tfrac{1}{2}g^{1/4}\Delta_2 g^{-1/4}.$$

Of course, in a parallel discussion of a chiral-invariant relativistic field theory, this B term is extremely divergent, being proportional to $(\delta^{(3)}(0))^2$. The manner whereby such terms might arise in such a theory is discussed by Dowker and Mayes (1973), and supports the need to include such terms in the expression for the action so that they might eventually cancel out in the evaluation of such quantities as S matrix elements. This theme is also discussed by Suzuki and Hattori (1972), who derive S matrix elements from the formula

$$S = T^*\exp\left(-\mathrm{i}\int \mathscr{H}'_{\mathrm{int}}(x)\,\mathrm{d}^4x\right)$$

with

$$\mathscr{H}'_{\mathrm{int}}(x) = -\{\mathscr{L}_{\mathrm{int}}\} + \delta\mathscr{H} + \delta'\mathscr{H}.$$

The term $\delta\mathscr{H}$, given by

$$\delta\mathscr{H} = \tfrac{1}{2}\mathrm{i}\delta^{(4)}(0)\ln g$$

is that which is needed to go from the group-invariant measure $\mathscr{D}(q)$ to the cartesian measure $d(q)$, as has already been indicated. The term $\{\mathscr{L}_{\mathrm{int}}\}$ is a symmetrized expression for the interaction lagrangian density, and $\delta'\mathscr{H}$ arises from symmetrizing the hamiltonian density; explicitly they have

$$\delta'\mathscr{H} = \tfrac{1}{8}(\delta^3(0))^2(g_{ab}g^{ac}_{,c}g^{bd}_{,d} - g^{cd}_{,cd}).$$

This term should, we assert, agree with our expression (4.30) for v. It does not, and the error can be traced to the fact that Suzuki and Hattori use as their lagrangian density

$$\mathscr{L} = \tfrac{1}{2}\partial_\mu\phi^a g_{ab}\partial^\mu\phi^b,$$

which is *not* chiral invariant if attention is paid to the order of factors. However, they go on to apply their result to an explicit calculation of contributions to the pion self-mass and to the pion–pion scattering amplitude, and show that with their choice of $\delta\mathscr{H}'$ the singular parts proportional to $(\delta^{(3)}(0))^2$ are exactly cancelled. To understand how this *correct* cancellation can come about even with the incorrect formula for $\delta\mathscr{H}'$, it is only necessary to remark that they do their calculation with the chiral transformations of the pion fields given by Weinberg (1968); that is, with

$$g_{ij} = \delta_{ij}(1+f_\pi^2\phi^2)^{-2}.$$

In this case our expression for v (modified as is appropriate for field theory by the inclusion of an additional factor $(\delta^{(3)}(0))^2$) and their expréssion for $\delta\mathscr{H}'$ agree, apart from a constant which has no effect on the amplitudes they calculate.

Finally we remark on a paper by Omote and Sato (1972), in which the canonical approach is used. We concur completely with their results, and have indeed used methods broadly comparable with theirs, in particular the resolution of ambiguities of ordering by the imposition of a symmetry.

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