ANNALS OF PHYSICS: 63, 586–591 (1971)

Quantum Mechanics with Constraints

H. JENSEN

Lehrstuhl für Theoretische Physik der Universität, 69 Heidelberg, Germany

AND

H. KOPPE

Institut für Theoretische Physik, Neue Universität, 2300 Kiel, Germany

Received September 9, 1970

The classical motion of a particle on a surface is simulated in quantum mechanics by forcing the particle to move between two parallel surfaces with distance d. In the limit $d \to 0$ one obtains an equation which differs from the equation proposed originally by Schrödinger by an additional potential depending on the curvature of the surface.

1. INTRODUCTION

In classical mechanics the motion subject to a constraint can be dealt with in a very elegant way using d'Alembert's principle. In the special case of holonomic constraints, one can reduce the degrees of freedom from the outset by writing down the Lagrangian equations with generalized coordinates q_λ representing the remaining degrees of freedom. One can consider this principle as an axiom, which is afterwards empirically justified by its successful application to technology. On the other hand, taking into account the fact, that no rod is really rigid, one can always argue, that a constraint of the form $\Phi(x, y, z) = 0$ is in reality produced by a potential energy $V_C = (C/2)\,\Phi^2$, where C is very large. One would then expect, to obtain d'Alembert's principle in the limit $C \to \infty$, so that for sufficiently large C d'Alembert's principle could be used as a reasonable approximative treatment of an otherwise rather complicated problem.

(As it turns out, the proof of this statement is by no means easy and only possible under suitable additional assumptions[1]).

Let us now turn to Quantum mechanics and consider the behaviour of a particle constrained to move on a surface $\Phi(x, y, z) = 0$. Since such systems do not exist,

[1] See a forthcoming paper in *Sitzungsber. Akad. Wiss. Heidelberg.*

this is not a physical problem, and we are at complete liberty to invent any mathematical formalism we like, without the risk of being reputed by experiment. One obvious choice, which has already been proposed by Schrödinger would be the following which largely corresponds to the procedure of Lagrange:

Introduce curvilinear coordinates u^λ ($\lambda = 1, 2$) with the metric

$$ds^2 = g_{\mu\nu}\, du^\mu\, du^\nu. \tag{1}$$

Define in the usual way $g^{\mu\nu}$ as the reciprocal of $g_{\mu\nu}$ and $g = \mathrm{Det}\, g_{\mu\nu}$. Then the Schrödinger equation is

$$-\frac{\hbar^2}{2M} g^{-\frac{1}{4}} \frac{\partial}{\partial u^\mu} g^{\mu\nu} g^{\frac{1}{4}} \frac{\partial \Psi}{\partial u^\nu} - V\Psi = E\Psi. \tag{2}$$

Since here simply the "second differential parameter" of differential geometry occurs in lieu of the Laplacian, this is an obvious choice.

It is therefore rather surprising, that, as shall be shown in this note, one obtains an equation different from Eq. (2) if one approaches the problem of constraints in a more realistic way by assuming that the particle is confined between two surfaces parallel to the surface $\Phi(x, y, z) = 0$ in a distance $\pm d/2$ and investigating the limit $d \to 0$. In this case, the energy of course contains the "zero point energy" $\epsilon_0 = \pi^2\hbar^2/2Md^2$, which goes to infinity if d goes to zero. What is of interest are the terms in E, which are of zero order in d, that is to say the limit

$$\epsilon = \lim_{d \to 0} \left(E - \frac{\pi^2\hbar^2}{2Md^2} \right). \tag{3}$$

It will turn out, that in this case, we obtain additional terms in (2) which correspond to a pseudopotential and depend on the curvature of the surface.

2. Motion on a Circle

As a preliminary example we shall discuss the two-dimensional motion of a particle confined to a annulus $R \leqslant r \leqslant R + d$. Introducing polar coordinates r and α and taking α as the one remaining degree of freedom, Eq. (2) would give

$$-\frac{\hbar^2}{2MR^2} \frac{\partial^2 \Psi}{\partial \alpha^2} = E\Psi$$

with the well-known eigenvalues

$$E = \frac{\hbar^2}{2MR^2} m^2 \qquad m = 0, \pm 1, \ldots . \tag{4}$$

On the other hand, one can start from the full equation

$$-\frac{\hbar^2}{2M}\left\{\frac{\partial^2\Psi}{\partial r^2}+\frac{1}{r}\frac{\partial\Psi}{\partial r}+\frac{1}{r^2}\frac{\partial^2\Psi}{\partial\alpha^2}\right\}=E\Psi \tag{5}$$

and solve it with the appropriate boundary conditions $\Psi = 0$ for $r = R$ and $r = R + d$. The solution can be written down in terms of Bessel functions of order m, and using the asymptotic developments one obtains in the limit $d \to 0$

$$E=\frac{\pi^2\hbar^2}{2Md^2}+\frac{\hbar^2}{2MR^2}\left[\left(m^2-\frac{1}{4}\right)+\frac{o}{(d)}\right], \tag{6}$$

and this differs from (4) by the term $-\hbar^2/8MR^2$.

We shall now try to obtain (6) directly from (5) without using the explicit form of the solution. Since we need the solution only in the narrow range $R < r < R + d$, it would be tempting to put $r = R$ in the second and third term on the left. The resulting equation with constant coefficients can be easily solved, the eigenvalues are

$$E=\frac{\pi^2\hbar^2}{2Md^2}+\frac{\hbar^2}{2MR^2}\left(m^2+\frac{1}{4}\right),$$

which differ from the correct values as given by (6) by the sign of the last term.

The reason, why the obvious simplification we introduced led to wrong results and was therefore not permissible is that we neglected terms of the form $(r - R)(\partial\Psi/\partial r)$. Now $r - R$ is of order d, whereas $\partial\Psi/\partial r$ is of order $1/d$, so that the whole term is of zero order in d and therefore not negligible. Therefore we can simplify (5) only after having transformed it into an equation, which does no longer contain terms, where a derivative with respect to r is multiplied by a function of r. This can be achieved by the substitution $\Psi = r^{-1/2}\chi$ which leads to the equation

$$-\frac{\hbar^2}{2M}\left\{\frac{\partial^2\chi}{\partial r^2}+\frac{1}{4r^2}\chi+\frac{1}{r^2}\frac{\partial^2\chi}{\partial\alpha^2}\right\}=E\chi. \tag{7}$$

In this equation, we can safely replace r by R, since by doing so we neglect only terms of order d, and then we obtain without difficulty the correct result given by (6) for the eigenvalues.

3. Motion between Equidistant Surfaces

We shall now treat the more general case, where the particle is confined to the space between two surfaces parallel in a distance $d/2$ to a given surface S. We assume, that the surface is given parametrically by

$$\mathbf{r} = \mathbf{a}(u^1, u^2). \tag{8}$$

Let $\mathfrak{n}(u^1, u^2)$ be the normal vector to the surface. We now introduce curvilinear coordinates u^1, u^2, τ by

$$\mathfrak{r} = \mathfrak{a}(u^1, u^2) + \mathfrak{n}\tau. \tag{9}$$

The surfaces $\tau = \text{const}$ are parallel surfaces to S, which itself is given by $\tau = 0$. The relation between x, y, z and u^1, u^2, τ is only unique for sufficiently small τ, since we are only interested in values $|\tau| < d/2$ with $d \to 0$ this is irrelevant. From (9) it follows, that

$$d\mathfrak{r} = \left(\frac{\partial \mathfrak{a}}{\partial u^1} + \tau \frac{\partial \mathfrak{n}}{\partial u^1}\right) du^1 + \left(\frac{\partial \mathfrak{a}}{\partial u^2} + \tau \frac{\partial \mathfrak{n}}{\partial u^2}\right) du^2 + \mathfrak{n}\, d\tau.$$

Since the derivatives of $\mathfrak{a}$ and $\mathfrak{n}$ with respect to the u^i are orthogonal to $\mathfrak{n}$, we obtain for the line-element

$$ds^2 = g_{ik} u^i u^k + (d\tau)^2, \tag{10}$$

with

$$g_{ik} = \left(\frac{\partial \mathfrak{a}}{\partial u^i} + \tau \frac{\partial \mathfrak{n}}{\partial u^i}\right)\left(\frac{\partial \mathfrak{a}}{\partial u^k} + \tau \frac{\partial \mathfrak{n}}{\partial u^k}\right). \tag{11}$$

We denote by $g(u^1, u^2, \tau)$ the determinant $\| g_{ik} \|$, and define a quantity γ by

$$g(u^1, u^2, \tau) = g(u^1, u^2, 0) \cdot \gamma \equiv g_0(u^1, u^2) \cdot \gamma. \tag{12}$$

It is an important property of γ, that it is invariant under a transformation of the u^i, since by such a transformation, g would be multiplied by the square of the Jacobian of the substitution independently of τ. We can therefore obtain γ by using an especially convenient system of parameters. If we choose the parameters in such a way, that $u^1 = \text{const}$ resp., $u^2 = \text{const}$ are lines of curvature on S, then we have the relations of Rodrigues

$$\frac{\partial \mathfrak{n}}{\partial u^i} = \frac{1}{R_i} \frac{\partial \mathfrak{a}}{\partial u^i},$$

where the R_i are the two principal radii of curvature of S. With this we obtain

$$\gamma = \left(1 + \frac{\tau}{R}\right)^2 \left(1 + \frac{\tau}{R_2}\right)^2. \tag{13}$$

After these preliminaries, we return to the Schrödinger equation and write it in the new variables

$$-\frac{\hbar^2}{2M}\left\{g^{-\frac{1}{4}}\frac{\partial}{\partial u^i}g^{ik}g^{\frac{1}{4}}\frac{\partial\Psi}{\partial u^k}+g^{-\frac{1}{4}}\frac{\partial}{\partial\tau}g^{\frac{1}{2}}\frac{\partial\Psi}{\partial\tau}\right\}=E\Psi. \tag{14}$$

If we check this equation for dangerous terms, where derivations with respect to τ are multiplied with functions of τ, we see, that they can only occur in the last term on the left,

$$g^{-\frac{1}{4}}\frac{\partial}{\partial\tau}g^{\frac{1}{4}}\frac{\partial\Psi}{\partial\tau}=\frac{\partial^2\Psi}{\partial\tau^2}+\frac{1}{2}\frac{\partial\log g}{\partial\tau}\frac{\partial\Psi}{\partial\tau},$$

$$=\frac{\partial^2\Psi}{\partial\tau^2}+\frac{1}{2}\frac{\partial\log\gamma}{\partial\tau}\frac{\partial\Psi}{\partial\tau}$$

(since g_0 does not depend on τ). If we put

$$\Psi=\gamma^{-1/4}\chi$$

we obtain

$$g^{-\frac{1}{4}}\frac{\partial}{\partial\tau}g^{\frac{1}{4}}\frac{\partial\Psi}{\partial\tau}=\gamma^{-\frac{1}{4}}\left(\frac{\partial^2\chi}{\partial\tau^2}+U\chi\right),$$

where

$$U=-\frac{1}{4}\frac{\partial^2\log\gamma}{\partial\tau^2}-\frac{1}{16}\left(\frac{\partial\log\gamma}{\partial\tau}\right)^2. \tag{15}$$

Equation (14) is then transformed into

$$-\frac{\hbar^2}{2M}\left\{\gamma^{\frac{1}{4}}g^{-\frac{1}{4}}\frac{\partial}{\partial u^i}g^{ik}g^{\frac{1}{4}}\frac{\partial}{\partial u^k}\gamma^{-\frac{1}{4}}\chi+\frac{\partial^2\chi}{\partial\tau^2}+U\chi\right\}=E\chi.$$

This does no longer contain any dangerous terms and one can put $\tau=0$ everywhere if one wants E only up to terms of zero order in the distance d of the enclosing surfaces. Since the condition for normalization is

$$\int|\Psi|^2 g_0^{\frac{1}{2}}\gamma^{\frac{1}{2}}\,du^1\,du^2\,d\tau=\int|\chi|^2 g_0^{\frac{1}{2}}\,du^1\,du^2\,d\tau,$$

the problem is separable and with

$$\chi=v(u^1,u^2)\left(\frac{2}{d}\right)^{\frac{1}{2}}\cos\frac{\pi\tau}{d}$$

we obtain for v Eq. (2) with the additional potential $-(\hbar^2/2M)U$. To obtain U, we have to insert (13) into (15) and put $\tau = 0$ in the final result. This gives

$$-\frac{\hbar^2}{2M}U = -\frac{\hbar^2}{8M}\left\{2\sum_i \frac{1}{R_i^2} - \left(\sum_i \frac{1}{R_i}\right)^2\right\}.$$

This result holds for any dimension; in ordinary space it can be simplified to

$$-\frac{\hbar^2}{2M}U = -\frac{\hbar^2}{8M}\left(\frac{1}{R_1} - \frac{1}{R_2}\right)^2.$$

This potential vanishes for a sphere, since in this case the two radii of curvature are equal. Therefore in this and only in this case, the realistic method gives the same result as the original prescription of Schrödinger.

References

1) E. Schrödinger, Ann. d. Physik **80** (1926), 489;
W. Pauli, in Handbuch der Physik, Bd 24/1 (Springer, Berlin, 1933) p. 120
2) A. K. Kerman, Mat. Fys. Medd. **30** nr. 15 (1956)
3) A. Faessler and W. Greiner, Z. Phys. **177** (1964) 190 and further references given there;
A. S. Davydov, Nucl. Phys. **24** (1961) 682;
A. S. Davydov and A. A. Chaban, Nucl. Phys. **20** (1960) 499
4) A. Bohr, Mat. Fys. Medd. **26** no. 14 (1952)
5) K. Kumar and M. Baranger, Nucl. Phys. **A122** (1968) 273 and the other papers on the pairing-plus-quadrupole model cited there
K. Kumar, Phys. Rev. **C1** (1970) 369
G. Gneuß, U. Mosel and W. Greiner, Phys. Lett. **31B** (1970) 269
6) J. Griffin, University of Maryland, Center for Theoretical Physics, Technical reports no. 805 (March 1968) and no. 810 (April 1968); Physics and Chemistry of Fission Symposium Vienna 1969, SM-122/200
7) J. R. Nix and W. J. Swiatecki, Nucl. Phys. **71** (1965) 1;
R. W. Hasse, Phys. Lett. **27B** (1968) 605
8) A. Sobiczewski, Z. Szymanski, S. Wycech, S. G. Nilsson, J. R. Nix, Ch. F. Tsang, C. Gustafson, P. Möller and B. Nilsson, Nucl. Phys. **A131** (1969) 60;
J. Damgaard, H. C. Pauli, V. M. Strutinski, C. Y. Wong, M. Brack, A. Stenholm-Jensen, Physics and Chemistry of Fission Symposium Vienna 1969, SM-122/62;
M. Brack, J. Damgaard, H. C. Pauli, A. Stenholm-Jensen, V. M. Strutinski and C. Y. Wong: "Funny Hills", to be submitted to Rev. Mod. Phys.
9) S. Flügge, Rechenmethoden der Quantentheorie (Springer Verlag, Heidelberg, 1965)
10) L. Wilets, Theories of nuclear fission (Clarendon Press, Oxford, 1964)
11) W. D. Myers and W. Swiatecki, Nucl. Phys. **81** (1966) 1
12) R. W. Hasse, private communication
13) V. M. Strutinski, Nucl. Phys. **A95** (1967) 420; Ark. Fys. **36** (1967) 629
14) J. E. Lynn, UKAEA Rep. AERE-R5891 (1968)
15) D. L. Hill and J. A. Wheeler, Phys. Rev. **83** (1953) 1102
16) E. Cheifetz, R. C. Jared, S. G. Thompson and J. B. Wilhelmy, Phys. Rev. Lett. **25** (1970) 38
17) P. Kienle, private communication
18) F. Weller, Fortschr. Phys., to be published
19) H. Jensen, H. Koppe, Ann. of Phys. **63** (1971); 586-591
H. Jensen, H. Koppe, forthcoming paper in Sitzungsber. Akad. Wiss. Heidelberg