MOMENTUM OPERATORS IN QUANTUM MECHANICS

by

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ABSTRACT

A representation for momentum operators corresponding to real observables is obtained by using functional integration in phase space.

1. Introduction

In quantum mechanics, real observables such as energy and momentum are represented by operators that are self-adjoint on the domain of physically acceptable bound state wave functions. A well-known example is provided by the form $P = -i\partial/\partial q$ for the momentum operator conjugate to coordinate q, where the domain is the entire real line R. However, if the domain is an interval $[\alpha, \beta]$ of R, a more general representation of P is necessary to ensure self-adjointness. One such general form for P has been suggested by Robinson and Hirschfelder [1], while an equivalent integral form, which can also be extended to functions of P has been proposed by Robinson and Lewis [2]. These forms were obtained in the context of conventional Schrödinger quantum mechanics.

An alternative way to define operators is possible, however, through an extension of the Feynman approach to quantum mechanics due to Davies [3]. In this work the equivalence of the Feynman and Schrödinger approaches was established by introducing a suitable inner product in function space. This inner product was defined for functions on $-\infty < q < \infty$, and the usual self-adjoint operators appropriate to this domain were therefore obtained. But the definition is readily extended to other domains , and hence can be used to obtain general self-adjoint representations for various operators. This is done here for any real function of P. The resulting representation leads to those given in [1] and [2].

2. Representation of operator $F(P)$

Following Davies [3] we introduce a function space with elements $f(q)$, $g(q)$, etc., which are here defined on the interval $[\alpha, \beta]$ of the real line. Then the appropriate inner product (f, g) is defined as follows:

$$(f, g) = \int_\alpha^\beta \bar{f}(q'') \left\{ \int_\alpha^\beta A(q'', T; q', 0)\, g(q')\, dq' \right\} dq'', \qquad (1)$$

where

$$A(q'', T; q', 0) = \int d[q(t)] \int d[p(t)/2\pi] \exp\left\{ i \int_0^T p\dot{q}\, dt \right\} \qquad (2)$$

is a functional integral over all phase space histories from $q(0) = q'$ to $q(T) = q''$, and involves only the <u>classical</u> variables p and q . If a division

$$0 = t_0 < t_1 < t_2 < \cdots < t_n = T \qquad (3)$$

of the time interval $(0, T)$ is made, and if

$$q_r = q(t_r), \quad p_r = p(\tau_r), \quad t_{r-1} \le \tau_r < t_r, \qquad (4)$$

then $A(q'', T; q', 0)$ is given by

$$A(q'';T;q',0) = \lim_{n\to\infty} \int_{-\infty}^{\infty} dq_1 \cdots \int_{-\infty}^{\infty} dq_{n-1} \int_{-\infty}^{\infty} \frac{dp_1}{2\pi} \cdots \int_{-\infty}^{\infty} \frac{dp_n}{2\pi}$$

$$\times \exp\left\{ i \sum_{r=1}^{n} p_r (q_r - q_{r-1}) \right\} . \tag{5}$$

This is readily evaluated and we find that

$$A(q'';T;q',0) = \delta(q''-q') , \tag{6}$$

where δ is the Dirac delta function. Thus the inner product (f,g) becomes

$$(f,g) = \int_{\alpha}^{\beta} \bar{f}(q'') \left\{ \int_{\alpha}^{\beta} \delta(q''-q')\, g(q')\, dq' \right\} dq''$$

$$= \int_{\alpha}^{\beta} \bar{f}(q)\, g(q)\, dq , \tag{7}$$

which is the frequently used inner product of function space.

Now we define the operator corresponding to a real function $F(P)$ of the momentum variable. This is done in terms of the inner product

$$(f,F(P)g) = \int_{\alpha}^{\beta} \bar{f}(q'') \left\{ \int_{\alpha}^{\beta} B(q'';T;q',0)\, g(q')\, dq' \right\} dq'' , \tag{8}$$

where

$$B(q'',T;q',0) = \int d[q(t)] \int d[p(t)/2\pi] \; F[p(\tau)] \exp\left\{ i \int_0^T p\dot{q}\, dt \right\}, \tag{9}$$

in which a time τ has been associated with $F[p(\tau)]$ such that $0 < \tau < T$, and once more the functional integration is over all phase space histories subject to the restrictions

$$q(0) = q', \qquad q(T) = q''. \tag{10}$$

Making the same division of the time interval $(0,T)$ as before, we may write $B(q'',T;q',0)$ as

$$B(q'',T;q',0) = \lim_{n\to\infty} \int_{-\infty}^{\infty} dq_1 \cdots \int_{-\infty}^{\infty} dq_{n-1} \int_{-\infty}^{\infty} \frac{dp_1}{2\pi} \cdots \int_{-\infty}^{\infty} \frac{dp_n}{2\pi} \times F(p_j) \exp\left\{ i \sum_{r=1}^{n} p_r (q_r - q_{r-1}) \right\}, \tag{11}$$

where $1 < j \leq n$. It is then found that

$$B(q'',T;q',0) = \hat{F}(q''-q'), \tag{12}$$

where

$$\hat{F}(q) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\xi q} F(\xi)\, d\xi. \tag{13}$$

Hence equation (8) becomes

$$(f, F(P)g) = \int_\alpha^\beta \bar{f}(q'') \left\{ \int_\alpha^\beta \hat{F}(q''-q') \, g(q') dq' \right\} dq'', \tag{14}$$

a result which is independent of the choice of τ and T. When $F(P) = I$, the identity operator, equation (14) reduces to (7) as it should.

The condition for $F(P)$ to be self-adjoint on the domain of the elements of the function space is

$$(f, F(P)g) = \overline{(g, F(P)f)} \tag{15}$$

Using (14) and the fact that F is a real function, we find that (15) implies the relation

$$\int_\alpha^\beta \bar{f}(q'') \left\{ \int_\alpha^\beta \hat{F}(q''-q') \, g(q') dq' \right\} dq''$$

$$= \int_\alpha^\beta \left\{ \int_\alpha^\beta \bar{f}(q'') \, \hat{F}(q''-q') \, dq'' \right\} g(q') dq', \tag{16}$$

that is, (14) is independent of the order of integration. Hence we may represent the self-adjoint operator $F(P)$ by the inner product

$$(f, F(P)g) = \int_\alpha^\beta \int_\alpha^\beta \bar{f}(q'') \, \hat{F}(q''-q') \, g(q') \, dq' dq'', \tag{17}$$

where

$$\hat{F}(q) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\xi q} F(\xi)\, d\xi\,, \tag{18}$$

subject to condition (16) for self-adjointness.

3. Alternative forms

Equation (17) may be written as

$$(f, F(P) g) = \int_{\alpha}^{\beta} \bar{f}(q'') \left\{ \int_{\alpha}^{\beta} \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\xi(q''-q')} F(\xi) d\xi \; g(q') dq' \right\} dq''$$

$$= \int_{\alpha}^{\beta} \bar{f}(q'') \left\{ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\xi q''} F(\xi) G(\xi)\, d\xi \right\} dq'', \tag{19}$$

where

$$G(\xi) = \frac{1}{\sqrt{2\pi}} \int_{\alpha}^{\beta} e^{-i\xi q'} g(q')\, dq'\,, \tag{20}$$

and where the order of the ξ and q' integrations has been interchanged. Hence $F(P)$ may be defined by

$$F(P) g(q) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\xi q} F(\xi) G(\xi)\, d\xi\,, \tag{21}$$

with $G(\xi)$ given by (20). This is the representation proposed by Robinson and Lewis [2] .

Next we consider the special case $F(P) = P$. This operator can be represented by the appropriate form of (21), but there is another form, which can be obtained directly from (17) and (18). For $F(P)=P$ equation (18) may be written as

$$\hat{F}(q) = -i\,\delta'(q)\,, \tag{22}$$

where δ' is the first derivative of the delta function. Hence (17) gives

$$(f, Pg) = -i \int_\alpha^\beta \int_\alpha^\beta \bar{f}(q'')\, \delta'(q''-q')\, g(q')\, dq'\, dq'' \tag{23}$$

$$\begin{aligned}
&= i \int_\alpha^\beta \bar{f}(q'') \left\{ \int_\alpha^\beta \frac{d\delta(q''-q')}{dq'}\, g(q')\, dq' \right\} dq'' \\
&= i \int_\alpha^\beta \bar{f}(q'')\, \delta(q''-\beta)\, dq''\, g(\beta) \\
&\quad - i \int_\alpha^\beta \bar{f}(q'')\, \delta(q''-\alpha)\, dq''\, g(\alpha) \\
&\quad + \int_\alpha^\beta \bar{f}(q) \left(-i\frac{\partial}{\partial q}\right) g(q)\, dq\,.
\end{aligned} \tag{24}$$

If we write

$$\int_\alpha^\beta \bar{f}(q)\, \delta(\beta-q)\, dq = \lambda \bar{f}(\beta)\,, \tag{25}$$

and

$$\int_{\alpha}^{\beta} \bar{f}(q)\,\delta(q-\alpha)\,dq = \mu \bar{f}(\alpha), \tag{26}$$

and impose condition (16) for self-adjointness, we find that

$$\lambda = \mu = \tfrac{1}{2} . \tag{27}$$

Thus (24) becomes

$$(f, Pg) = \int_{\alpha}^{\beta} \bar{f}(q) \left(-i\frac{\partial}{\partial q}\right) g(q)\,dq + \tfrac{1}{2} i \left\{ \bar{f}(\beta) g(\beta) - \bar{f}(\alpha) g(\alpha) \right\} . \tag{28}$$

Defining $\delta_-(\beta-q)$ and $\delta_+(q-\alpha)$ by the relations

$$\int_{u}^{\beta} f(q)\,\delta_-(\beta-q)\,dq = f(\beta), \qquad \alpha \le u < \beta, \tag{29}$$

$$\int_{\alpha}^{v} f(q)\,\delta_+(q-\alpha)\,dq = f(\alpha), \qquad \alpha < v \le \beta, \tag{30}$$

we may write (28) in the form

$$(f, Pg) = \int_{\alpha}^{\beta} \bar{f}(q) \left\{ -i\frac{\partial}{\partial q} + \tfrac{1}{2} i \delta_{-}(\beta - q) - \tfrac{1}{2} i \delta_{+}(q - \alpha) \right\} g(q)\, dq, \quad (31)$$

or

$$P = -i\frac{\partial}{\partial q} + \tfrac{1}{2} i \delta_{-}(\beta - q) - \tfrac{1}{2} i \delta_{+}(q - \alpha). \quad (32)$$

This is the representation of P suggested by Robinson and Hirschfelder [1] using quite a different set of considerations.

4. Concluding remarks

A representation for real functions of the momentum operator P has been obtained by using functional integration in phase space. The resulting operators are self-adjoint on the interval $[\alpha, \beta]$ of the real line. For the operator P itself, the representation involves the first derivative of the delta function, in agreement with the treatment of momentum given by Kramers [4] .

The present work has dealt solely with cartesian coordinates. It would be of interest to extend the method to other coordinate systems, though this may prove difficult in the light of work by Edwards and Gulyaev [5] on functional integrals in polar coordinates.

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I should like to thank Professor J. O. Hirschfelder and Professor B. Noble for helpful discussions on this subject.

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1. Introduction

In quantum mechanics, real observables such as energy and momentum are represented by operators that are self-adjoint on the domain of physically acceptable bound state wave functions. A well-known example is provided by the form $P = -i\,\partial/\partial q$ for the momentum operator conjugate to coordinate q, which is self-adjoint on the real line $(-\infty, \infty)$. However, if the domain is an interval $[\alpha, \beta]$ of the real line, a more general representation of P is necessary to ensure self-adjointness. One such general form for P has been suggested by Robinson and Hirschfelder [1], while an equivalent integral form, which can also be extended to functions of P, has been proposed by Robinson and Lewis [2]. These forms were presented in the context of conventional Schrödinger quantum mechanics.

An alternative way to define operators is possible, however, through an extension of the Feynman approach to quantum mechanics due to Davies [3]. In this work the equivalence of the Feynman and Schrödinger approaches was established by introducing a suitable inner product in function space. This inner product was defined for functions on the real line, and the usual self-adjoint operators appropriate to this domain were therefore obtained. But the definition is readily extended to other domains, and hence can be used to obtain

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general self-adjoint representations for various operators. This is done here for any real function of P. The resulting representation leads to those given in [1] and [2].

2. The inner product

Following Davies [3] we introduce a function space with elements $f(q)$, $g(q)$, etc., which are here defined on the interval $[\alpha, \beta]$ of the real line. Then the inner product (f, g) is defined as follows:

$$(f, g) = \int_{\alpha}^{\beta} \bar{f}(q'') \left\{ \int_{\alpha}^{\beta} A(q'', T; q', 0)\, g(q')\, dq' \right\} dq'' \quad , \tag{1}$$

where

$$A(q'', T; q', 0) = \int d[q(t)] \int d[p(t)/2\pi] \exp\left\{ i \int_{0}^{T} p\dot{q}\, dt \right\} \tag{2}$$

is a functional integral over all phase space histories from $q(0) = q'$ to $q(T) = q''$, and involves only the classical variables p and q. If a division

$$0 = t_0 < t_1 < t_2 < \ldots < t_n = T \tag{3}$$

of the time interval $(0, T)$ is made, and if

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This is readily evaluated and we find that

$$A(q'', T; q', 0) = \lim_{n \to \infty} \delta(q_n - q_0) \;, \tag{6}$$

where δ is the Dirac delta function. Now $q_o = q'$ and $q_n = q''$, and hence

$$A(q'', T; q', 0) = \delta(q'' - q') , \tag{7}$$

a result independent of T. Thus the inner product (f, g) becomes

$$(f, g) = \int_\alpha^\beta \bar{f}(q'') \{ \int_\alpha^\beta \delta(q'' - q') g(q') dq' \} dq''$$

$$= \int_\alpha^\beta \bar{f}(q) g(q) dq , \tag{8}$$

which is the frequently used inner product of function space.

3. Representation of operator F(P).

Now we define the operator corresponding to a real function $F(p)$ of the momentum variable. This is done in terms of the inner product

$$(f, F(P)g) = \int_\alpha^\beta \bar{f}(q'') \{ \int_\alpha^\beta B(q'', T; q', 0) g(q') dq' \} dq'' , \tag{9}$$

where

$$B(q'', T; q', 0) = \int d[q(t)] \int d[p(t)/2\pi] F[p(\tau)] \exp \{ i \int_0^T p\dot{q} dt \} , \tag{10}$$

in which a time τ has been associated with $F[p(\tau)]$ such that $0 < \tau < T$, and once more the functional integration is over all phase space histories subject to the restrictions

$$q(0) = q' , \quad q(T) = q'' . \tag{11}$$

Making the same division of the time interval $(0, T)$ as before, we may write $B(q'', T; q', 0)$ as

$$B(q'', T; q', 0) = \lim_{n \to \infty} \int_{-\infty}^{\infty} dq_1 \cdots \int_{-\infty}^{\infty} dq_{n-1} \int_{-\infty}^{\infty} \frac{dp_1}{2\pi} \cdots \int_{-\infty}^{\infty} \frac{dp_n}{2\pi}$$

$$F(p_j) \exp \{ i \sum_{r=1}^{n} p_r (q_r - q_{r-1}) \} , \tag{12}$$

where j is an integer such that $1 < j \leq n$. It is then found that

$$B(q'', T; q', 0) = \hat{F}(q'' - q') \quad , \tag{13}$$

where

$$\hat{F}(q) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\xi q} F(\xi)\, d\xi \quad . \tag{14}$$

Hence equation (11) becomes

$$(f, F(P) g) = \int_{\alpha}^{\beta} \bar{f}(q'') \left\{ \int_{\alpha}^{\beta} \hat{F}(q'' - q') g(q') dq' \right\} dq'' \quad , \tag{15}$$

a result which is independent of τ and T. When $F(P)$ is equal to the identity operator, equation (15) reduces to (8), as it should.

The condition for $F(P)$ to be self-adjoint on the interval $[\alpha, \beta]$ is

$$(f, F(P)g) = \overline{(g, F(P) f)} \quad . \tag{16}$$

Using (15) and the fact that F is a real function, we find that (16) implies the relation

$$\int_{\alpha}^{\beta} \bar{f}(q'') \left\{ \int_{\alpha}^{\beta} \hat{F}(q'' - q') g(q') dq' \right\} dq'' = \int_{\alpha}^{\beta} \left\{ \int_{\alpha}^{\beta} \bar{f}(q'') \hat{F}(q'' - q') dq'' \right\} g(q')\, dq' \quad , \tag{17}$$

that is, (15) is independent of the order of integration. Hence we may represent the self-adjoint operator $F(P)$ by the inner product

$$(f, F(P) g) = \int_{\alpha}^{\beta} \int_{\alpha}^{\beta} \bar{f}(q'') \hat{F}(q'' - q') g(q') dq'\, dq'' \quad , \tag{18}$$

where

$$\hat{F}(q) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\xi q} F(\xi)\, d\xi \tag{19}$$

subject to condition (17) for self-adjointness.

4. Alternative forms.

Equation (18) may be written as

$$(f, F(P)g) = \int_\alpha^\beta \bar{f}(q'') \{ \int_\alpha^\beta \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\xi(q''-q')} F(\xi) d\xi\, g(q')\, dq' \}\, dq''$$

$$= \int_\alpha^\beta \bar{f}(q'') \{ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\xi q''} F(\xi) G(\xi)\, d\xi \}\, dq'' \quad , \tag{20}$$

in which

$$G(\xi) = \frac{1}{\sqrt{2\pi}} \int_\alpha^\beta e^{-i\xi q'} g(q')\, dq' \quad , \tag{21}$$

and where we have interchanged the order of the ξ and q' integrations. Hence $F(P)$ may be defined by

$$F(P)g(q) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\xi q} F(\xi) G(\xi)\, d\xi \quad , \tag{22}$$

with $G(\xi)$ given by (21). This is the representation proposed by Robinson and Lewis [2].

Next we consider the special case $F(P) = P$. This operator can be represented by the appropriate form of (22), but there is another form, which can be obtained directly from (18) and (19). For $F(P) = P$, equation (19) may be written as

$$\hat{F}(q) = -i\,\delta'(q) \quad , \tag{23}$$

where δ' is the first derivative of the delta function. Hence (18) gives

$$(f, Pg) = -i \int_\alpha^\beta \int_\alpha^\beta \bar{f}(q'')\, \delta'(q''-q')\, g(q')\, dq'\, dq'' \tag{24}$$

$$= i \int_\alpha^\beta \bar{f}(q'') \{ \int_\alpha^\beta \frac{d\delta(q''-q')}{dq'} g(q')\, dq' \}\, dq''$$

$$= i \int_\alpha^\beta \bar{f}(q'')\, \delta(q''-\beta)\, dq''\, g(\beta) - i \int_\alpha^\beta \bar{f}(q'')\, \delta(q''-\alpha)\, dq''\, g(\alpha)$$

$$+ \int_\alpha^\beta \bar{f}(q) \left(-i \frac{\partial}{\partial q}\right) g(q)\, dq \quad . \tag{25}$$

If we write

$$\int_{\alpha}^{\beta} \bar{f}(q)\,\delta(\beta - q)\,dq = \lambda \bar{f}(\beta) , \tag{26}$$

and

$$\int_{\alpha}^{\beta} \bar{f}(q)\,\delta(q - \alpha)\,dq = \mu \bar{f}(\alpha) , \tag{27}$$

and impose condition (17) for self-adjointness, we find that

$$\lambda = \mu = \frac{1}{2} . \tag{28}$$

Thus (25) becomes

$$(f, Pg) = \int_{\alpha}^{\beta} \bar{f}(q)\left(-i\frac{\partial}{\partial q}\right) g(q)dq + \tfrac{1}{2} i \{ \bar{f}(\beta)g(\beta) - \bar{f}(\alpha)g(\alpha) \} . \tag{29}$$

Defining $\delta_{-}(\beta-q)$ and $\delta_{+}(q-\alpha)$ by the relations

$$\int_{u}^{\beta} f(q)\delta_{-}(\beta - q)\,dq = f(\beta) , \qquad \alpha \leq u < \beta , \tag{30}$$

$$\int_{\alpha}^{\nu} f(q)\,\delta_{+}(q - \alpha)dq = f(\alpha) , \qquad \alpha < \nu \leq \beta , \tag{31}$$

we may write (29) in the form

$$(f, Pg) = \int_{\alpha}^{\beta} \bar{f}(q) \{ -i\frac{\partial}{\partial q} + \tfrac{1}{2} i\,\delta_{-}(\beta - q) - \tfrac{1}{2} i\,\delta_{+}(q - \alpha) \} g(q)\,dq , \tag{32}$$

or

$$P = -i\frac{\partial}{\partial q} + \tfrac{1}{2} i\,\delta_{-}(\beta - q) - \tfrac{1}{2} i\,\delta_{+}(q - \alpha) . \tag{33}$$

This is the representation of P suggested by Robinson and Hirschfelder [1] using quite a different set of considerations.

5. Concluding remarks.

A representation for real functions of the momentum operator P has been obtained by using functional integration in phase space. The resulting operators are self-adjoint on the interval $[\alpha, \beta]$ of the real line. For the operator P itself, the representation involves the first derivative of the delta function, in agreement with the treatment of momentum given by Kramers [4]. Some related work on operators, from quite a different standpoint, can also be found in a paper by Fuchs [5].

The present work has dealt solely with cartesian coordinates. It would be of interest to extend the method to other coordinate systems, though this may prove difficult in the light of work by Edwards and Gulyaev [6] on functional integrals in polar coordinates.

I should like to thank Professor J. O. Hirschfelder and Professor B. Noble for helpful discussions on this subject, and Professor C. A. Coulson for bringing the paper of Fuchs to my attention.

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