# Resolution of the Operator-Ordering Problem by the Method of Finite Elements

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The method of finite elements converts the operator Heisenberg equations that arise from a Hamiltonian of the form $H=P^2/2+V(q)$ into a set of operator difference equations on a lattice. The equal-time commutation relations are exactly preserved and thus are consistent with the requirements of unitarity. We consider general Hamiltonians of the form $H(p,q)$ and show that the requirement of unitarity uniquely determines the operator ordering in such Hamiltonians. (The ordering procedure involves a set of orthogonal polynomials which are not widely known.) Our result shows that it is possible to treat quantum spin systems by the method of finite elements.

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In this Letter we consider Hamiltonians of the form $H=H(p,q)$. We address the problem of converting the operator differential equations of motion

$$\dot{q}(t)=\frac{\partial H}{\partial P}=\frac{1}{i}[q,H],\qquad \dot{p}(t)=-\frac{\partial H}{\partial q}=\frac{1}{i}[p,H] \tag{1}$$

into a system of unitary-operator difference equations on a time lattice. By the term unitary we mean that the difference equations exactly preserve the equal-time commutation relations

$$[q(t),p(t)]=i \tag{2}$$

at each time step. We show that if the method of finite elements is used to construct the operator difference equations[1] then the ordering of the operators $p$ and $q$ appearing in the Hamiltonian $H(p,q)$ is uniquely determined by the requirement of unitarity.

The method of linear finite elements approximates the operators $q(t)$ and $p(t)$ by a time sequence of operators $q_n$ and $p_n$ $(n=0,1,2,\ldots)$, where $t=nh$ and $h$ is the lattice spacing. The method consists of making the replacements

$$\dot{q}(t)\to(q_{n+1}-q_n)/h,\quad \dot{p}(t)\to(p_{n+1}-p_n)/h,\qquad q(t)\to q_n+q_{n+1})/2,\quad p(t)\to(p_n+p_{n+1})/2 \tag{3}$$

in (1). The derivation of (3) is given in Ref. 1.

Thus, on the lattice, the differential equations (1) become

$$\dot{Q}=\frac{\partial}{\partial P}H(P,Q),\quad \dot{P}=-\frac{\partial}{\partial Q}H(P,Q), \tag{4}$$

where we have used the notation

$$\dot{Q}\equiv(q_{n+1}-q_n)/h,\quad \dot{P}\equiv(p_{n+1}-p_n)/h,\qquad Q=(q_n+q_{n+1})/2,\quad P=(p_n+p_{n+1})/2. \tag{5}$$

To establish unitarity one must prove that

$$[q_{n+1},p_{n+1}]=[q_n,p_n]\quad(n=0,1,2,\ldots). \tag{6}$$

We can establish (6) if we can explicitly show from the operator difference equations (4) that

$$[\dot{Q},P]+[Q,\dot{P}]=0. \tag{7}$$

To see this we substitute the definitions in (5) into (7) and expand the commutators; this calculation directly shows that (7) implies (6). Thus, our objective is to examine the expression

$$\left[\frac{\partial}{\partial P}H(P,Q),P\right]-\left[Q,\frac{\partial}{\partial Q}H(P,Q)\right] \tag{8}$$

and to show that it vanishes.

It is crucial to remark that in general (8) does *not* vanish. This is because the commutator

$$\theta\equiv[Q,P] \tag{9}$$

is not a $c$ number even though $[q(t),p(t)]$ is; the quantity $\theta$ is an operator because it contains the unequal-time commutators $[q_n,p_{n+1}]$ and $[q_{n+1},p_n]$.

To investigate (8) we may assume that $H$ is Hermitian and that $H(P,Q)$ can be expanded in a series of Hermitian terms $H_{m,n}(P,Q)$, where $H_{m,n}$ $(m,n\geq 0)$ is a sum of monomials containing $m$ factors of $P$ and $n$ factors of $Q$. We can examine each term $H_{m,n}$ of the series independently. For example, $H_{2,2}$ has the form

$$H_{2,2}=aPQ^2P+bQP^2Q+c(P^2Q^2+Q^2P^2)+d(PQPQ+QPQP), \tag{10}$$

where $a$, $b$, $c$, and $d$ are real constants. To illustrate our procedure we examine $H_{2,2}$ in detail. We compute

$$\left[\frac{\partial}{\partial P}H_{2,2},P\right]-\left[Q,\frac{\partial}{\partial Q}H_{2,2}\right] = (2c-a-d)(\theta QP+PQ\theta)+(a-b)(Q\theta P+P\theta Q)+(b+d-2c)(\theta PQ+QP\theta). \quad (11)$$

Thus, unitarity requires that $2c-a-d=0$, $a-b=0$, $b+d-2c=0$. The solution to these equations is $a=b$ and $d=2c-b$, where $b$ and $c$ are arbitrary real constants. Thus, it appears that there is a two-parameter family of Hamiltonians of the type $H_{2,2}$ which satisfy unitarity on the lattice. Indeed, $H_{2,2}$ can be written in the form

$$H_{2,2}=cT_{2,2}+(c-b)G_{2,2}, \quad (12)$$

where

$$T_{2,2}(P,Q)=PQ^2P+QP^2Q+P^2Q^2+Q^2P^2+PQPQ+QPQP \quad (13)$$

and

$$G_{2,2}(P,Q) = PQPQ+QPQP-QP^2Q-PQ^2P. \quad (14)$$

Thus, if we were given a *continuum* Hamiltonian of the general form $H_{2,2}(p,q)$ we could reorder the operators $p$ and $q$ [using the commutation relation (2)] to make it take the form in (12) before making the finite-element transcription (3). [This reordering of operators of course produces additional simpler terms of the form $H_{1,1}=a(pq+qp)$.] However, we observe that $G_{2,2}(p,q)$ is trivial; using (2) we see that $G_{2,2}(p,q)=-1$. The above calculation shows that the requirement of lattice unitarity forces us to preorganize the operators $p$ and $q$ in $H_{2,2}(p,q)$ in a *unique* way; namely, the totally symmetric sum ($T$ form) in (13). For example, if we are given the Hamiltonian $H_{2,2}(p,q)=5qp^2q$, this Hamiltonian must be (uniquely) reordered by use of (2) as

$$H_{2,2}(p,q)=\tfrac{5}{6}T_{2,2}(p,q)+\tfrac{5}{2} \quad (15)$$

before going onto the lattice by use of (3).

What is remarkable is that given *any* Hamiltonian $H_{m,n}(q,p)$ carrying out the above procedure shows that there is always a *unique* form which is necessary and sufficient in order that the equal-time commutators be preserved as in (6). In particular, we must rewrite

$$H_{m,n}(p,q)=\alpha T_{m,n}(p,q)+H_{m-2,n-2}(p,q), \quad (16)$$

where $T_{m,n}$ is the totally symmetric sum ($T$ form) of all possible monomials containing $m$ factors of $p$ and $n$ factors of $q$. This process is then iterated until $H_{m,n}$ is a descending sum of totally symmetric parts:

$$H_{m,n}(p,q) =\alpha T_{m,n}(p,q)+\beta T_{m-2,n-2}(p,q)+\ldots . \quad (17)$$

To verify this assertion we must use the fact that derivatives leave the $T$ form intact. In fact we have the identities

$$\frac{\partial}{\partial P}T_{m,n}(P,Q)=(m+n)T_{m-1,n}(P,Q),$$
$$\frac{\partial}{\partial Q}T_{m,n}(P,Q)=(m+n)T_{m,n-1}(P,Q). \quad (18)$$

In addition, we observe that commutators maintain the totally symmetric form:

$$[Q,T_{m,n}(P,Q)]=T_{m-1,n,1}(P,Q,\theta),$$
$$[T_{m,n}(P,Q),P]=T_{m,n-1,1}(P,Q,\theta), \quad (19)$$

where $T_{m,n,1}(P,Q,\theta)$ is the totally symmetric sum of all monomials having $m$ factors of $P$, $n$ factors of $Q$, and one factor of $\theta$. Using (18) and (19) it is easy to verify that the expression in (8) vanishes when $H(P,Q)$ is in $T$ form.

This ordering procedure applies to all Hamiltonians $H(p,q)$ which are polynomials in the variables $p$ and $q$. However, if $H$ is a nonpolynomial function the ordering problem is much more challenging. For example, consider a class of Hamiltonians of the form

$$H(p,q)=H(T_{1,1})=H(pq+qp). \quad (20)$$

To order the operators of this Hamiltonian we introduce a little-known set of orthonormal polynomials $S_n(x)$ called continuous Hahn polynomials.[2] These polynomials emerge from the simple observation that $T_{n,n}$ is a polynomial function of $T_{1,1}$; the defining equation for $S_n(x)$ is therefore[3]

$$S_n(T_{1,1})\equiv T_{n,n}/(2n-1)!!. \quad (21)$$

The first few polynomials $S_n(x)$ are

$$S_0(x)=1,\quad S_1(x)=x,\quad S_2(x)=\tfrac{1}{2}(x^2-1),$$
$$S_3(x)=\tfrac{1}{6}(x^3-5x),\quad S_4(x)=\tfrac{1}{24}(x^4-14x^2+9),$$
$$S_5(x)=\tfrac{1}{120}(x^5-30x^3+89x),$$
$$S_6(x)=\tfrac{1}{720}(x^6-55x^4+439x^2-225).$$

These polynomials have the following properties[4]: (i) The generating function $G(t)$ is

$$G(t)=\frac{e^{x\arctan t}}{(1+t^2)^{1/2}}=\sum_{n=0}^{\infty}S_n(x)t^n. \qquad (22)$$

(ii) The orthonormality condition is

$$\int_{-\infty}^{\infty}dx\, w(x)S_m(x)S_n(x)=\delta_{mn}, \qquad (23)$$

where the weight function $w(x)$ is given by[5]

$$w(x)=[2\cosh(\pi x/2)]^{-1}. \qquad (24)$$

(iii) A recursion relation satisfied by $S_n(x)$ is

$$nS_n(x)=xS_{n-1}(x)-(n-1)S_{n-2}(x). \qquad (25)$$

The polynomials do not satisfy a second-order differential equation but they do obey the second-order functional difference eigenvalue equation

$$(1-ix)S_n(x+2i)+(1+ix)S_n(x-2i)=(4n+2)S_n(x). \qquad (26)$$

Now we return to the problem of ordering the operator $H$ in (20). Using the completeness of $S_n(x)$ we expand $H(x)$ as a series in $S_n(x)$:

$$H(x)=\sum_{n=0}^{\infty}a_nS_n(x), \qquad (27)$$

where

$$a_n=\int_{-\infty}^{\infty}dx\, w(x)H(x)S_n(x). \qquad (28)$$

Thus, from (21) we have

$$H(T_{1,1})=\sum_{n=0}^{\infty}a_nT_{n,n}/(2n-1)!!. \qquad (29)$$

We have therefore represented $H(pq+qp)$ as an infinite sum of operators in $T$ form. In the form (29) $H$ is directly amenable to lattice transcription and the resulting operator difference equations automatically preserve unitarity.

As an example, consider the Hamiltonian $H=e^{c(pq+qp)}$, where $c$ is a constant. For the exponential function, the integral in (28) can be performed in closed form and the result is $a_n=(\tan c)^n[1+(\tan c)^2]^{1/2}$. Thus,

$$H=[1+(\tan c)^2]^{1/2}\sum_{n=0}^{\infty}(\tan c)^nS_n(pq+qp)$$
$$=[1+(\tan c)^2]^{1/2}\sum_{n=0}^{\infty}\frac{(\tan c)^n}{(2n-1)!!}T_{n,n}.$$

$H$ is now in its *unique* $T$ form and therefore the resulting Heisenberg equations can be transcribed onto the lattice.

An interesting and attractive application of this analysis concerns spin systems. Although the finite-element method is applicable to and useful for a variety of problems in quantum mechanics and field theory,[6] all these problems are described by Hamiltonians whose variables satisfy the Neumann or Heisenberg algebra $[q,p]=i$. However, there are other important Hamiltonians in physics whose variables belong to other algebras. For example, the Hamiltonian $H=H(S_x,S_y,S_z)$, where $\mathbf{S}$ satisfies the SU(2) algebra, has not yet been studied in the finite-element approximation.

There is a simple and direct way to transcribe the operator difference equations of such systems onto a lattice. One can use any of several transformations: the Holstein-Primakoff, Schwinger, Maleev, and Villain transformations express the spin operators in terms of elements of a Heisenberg algebra.[7] For example, the Maleev transformation is

$$S_+=\frac{p+iq}{4\sqrt{s}}(4s+1-p^2-q^2),$$
$$S_-=\sqrt{s}\,(p-iq), \qquad (30)$$
$$S_z=\tfrac{1}{2}(p^2+q^2-1-2s),$$

where $\mathbf{S}^2=s(s+1)$. Transformations such as that in (30) share a common problem in that they convert spin Hamiltonians into Hamiltonians of the general form $H(p,q)$ whose operators are not properly ordered. We have shown in this paper that *all* such Hamiltonians have a *unique* operator reordering that facilitates their analysis by the method of finite elements. We emphasize that our reordering prescription does *not* change the physics of the Hamiltonian, but it is essential for the mathematical consistency of the operator difference equations.

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[3]This definition of $S_n(x)$ in (21) very closely resembles that of the Chebyshev polynomials $T_n(x)$. Using the fact that $\cos(n\theta)$ is a polynomial in $\cos\theta$ one defines $T_n(\cos\theta)\equiv\cos(n\theta)$. The same polynomials $S_n(x)$ occur in the expansion of $T_{m,n}$. The generalization of (21) is

$$T_{m,m+k}=\frac{(2m+k)!}{(m+k)!2^{m+1}}\{q^k,S_m(T_{1,1})\}_+.$$

[4]A detailed description of these new polynomials will be

given elsewhere.

[5]There is an interesting connection between these polynomials and the Euler numbers $E_n$: $\int_{-\infty}^{\infty} dx\, w(x) x^{2n} = |E_{2n}|$.

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