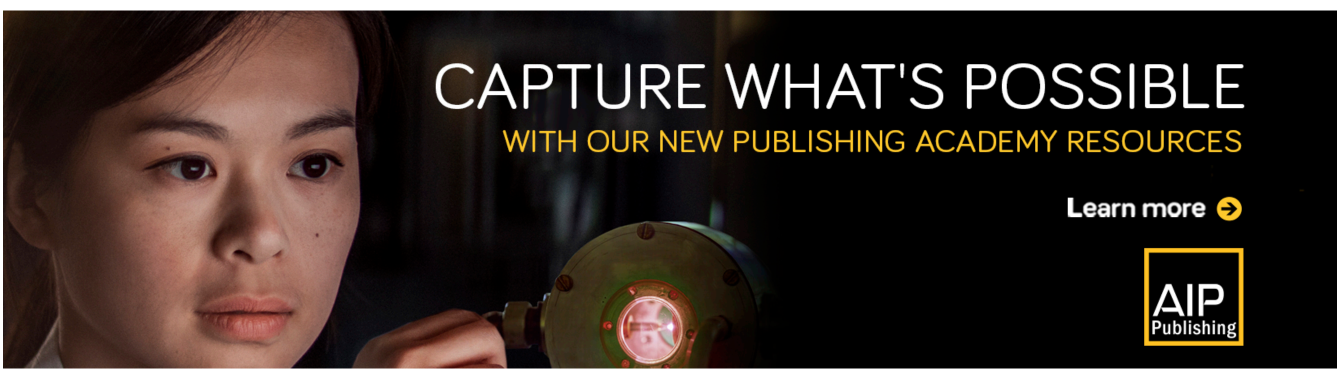
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Self-adjointness and spontaneously broken symmetry

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(Received 23 February 1977; accepted 20 April 1977)

The notion of self-adjointness as distinct from Hermiticity is usually avoided in elementary quantum mechanics courses due to a feeling that it has nothing to do with physics or else is too mathematical. This is definitely not the case, and we use the model of a free particle restricted to motion on a line over a finite interval, to demonstrate this. For such a particle, there is one-parameter infinity of self-adjoint extensions of the momentum operator. We use one of these, corresponding to "antiperiodic" boundary conditions, to show that physical phenomena different from the usual case (periodic boundary conditions) occur. In fact, in this case, we have a model displaying many of the properties of spontaneously broken symmetry.

I. INTRODUCTION

In most introductory courses on quantum mechanics there is a chapter on operators. Usually, it is pointed out that operators corresponding to observables should be Hermitian; the difference between Hermitian and self-adjoint is usually not even mentioned.[1] This is probably due to a feeling that such a distinction is only nitpicking and has nothing to do with physics.

It is the purpose of this note to illustrate that the distinction between Hermitian and self-adjoint is really physical and not just mathematical pedantry. To illustrate this, we shall use a free particle confined to a finite interval on a line. By taking a self-adjoint extension different from the usual one, we are able to display some interesting and surprising properties of this system.

II. SELF-ADJOINTNESS FOR A PARTICLE ON AN INTERVAL

We consider a free particle defined on the interval $-a \leq x \leq a$. The Hamiltonian for this particle is

$$H = p^2/2m, \tag{1}$$

where as usual the momentum operator p is represented by

$$p = \frac{\hbar}{i}\frac{d}{dx}. \tag{2}$$

As it stands, this operator p is Hermitian, but not necessarily self-adjoint. This is easily seen by computing

$$\begin{aligned}(f,pg) - (pf,g) &= \int_{-a}^{a}\left[f^*\frac{\hbar}{i}\frac{dg}{dx} - \left(\frac{\hbar}{i}\frac{df}{dx}\right)^* g\right]dx \\ &= \frac{\hbar}{i}\,[f^*(a)g(a) - f^*(-a)g(-a)]. \end{aligned} \tag{3}$$

Thus, $(f,pg) = (pf,g)$ and p is self-adjoint if and only if

$$[f(a)/f(-a)]^* = g(-a)/g(a). \tag{4}$$

This is satisfied by requiring

$$f(a) = e^{i\alpha 2\pi}f(-a), \qquad 0 \leq \alpha < 1 \tag{5}$$

for all functions f in the domain of p.

For each value of α we now get a different self-adjoint momentum operator p_α. The usual procedure is to take periodic boundary conditions namely $\alpha = 0$. This choice has definite physical implications and should be justified since a different choice of α leads to different physical results. A possible justification is that periodic boundary conditions have a simple infinite-volume limit.

Before proceeding to a discussion of our specific model we still need a definition of broken symmetry. There are two separate cases: discrete and continuous symmetries.

Suppose we have an operator Q which generates a symmetry operation, either discrete-like parity or time-reversal Q_D, or else continuous Q_C. Suppose further, that Q commutes with the Hamiltonian H of the system. Then using Q_C one can form the unitary operator

$$U(\alpha) = e^{i\alpha Q_C}, \tag{6}$$

and

$$[Q,H] = 0 \tag{7}$$

yields

$$U(\alpha)HU^\dagger(\alpha) = H, \tag{8}$$

or

$$Q_D H Q_D^{-1} = H. \tag{9}$$

If, furthermore, the ground state $|0\rangle$ of the Hamiltonian is invariant under Q_D or $U(\alpha)$, i.e.,

$$Q_D|0\rangle = |0\rangle \tag{10}$$

or

$$U(\alpha)|0\rangle = |0\rangle, \tag{11}$$

then Q generates a symmetry of the system.

Conversely, we define a symmetry corresponding to an operation Q to be spontaneously broken if the ground state is not an eigenstate of Q. This means neither Eq. (10) nor Eq. (11) are true. For this to occur requires that the ground state be degenerate—in itself an unusual phenomenon.

III. THE MODEL

We use the Hamiltonian Eq. (1) with the momentum operator given by Eq. (2) and domain of the operator $\mathcal{D}_p$ defined by $\mathcal{D}_p = \{f(x)$, twice continuously differentiable and such that $f(a) = -f(-a)\}$. Thus, instead of periodic, we pick "antiperiodic" boundary conditions. We have, in fact, chosen $\alpha = \frac{1}{2}$.[2]

The complete set of normalized eigenfunctions of this momentum operator are given by

$$f_n(x) = (2a)^{-1/2} \exp[i\pi(n + \tfrac{1}{2})x/a], \quad n = 0,\pm1,\pm2,\ldots, \qquad (12)$$

with corresponding eigenvalues $(\pi\hbar/a)(n + \tfrac{1}{2})$.

These wave functions have the following symmetry properties:

$$f_n(x) = f_{-(n+1)}(-x), \qquad (13)$$

$$f_n^*(x) = f_{-(n+1)}(x). \qquad (14)$$

Thus, the parity operator P and the time-reversal operator T have the following action on them:

$$(Pf_n)(x) = f_{-(n+1)}(x), \qquad (15)$$

$$(Tf_n)(x) = f_{-(n+1)}(x). \qquad (16)$$

The set of functions $\{f_n\}$ are also eigenfunctions of the Hamiltonian. In fact,

$$Hf_n = (\pi^2\hbar^2/2ma^2)(n + \tfrac{1}{2})^2 f_n, \qquad (17)$$

$$Hf_{-(n+1)} = (\pi^2\hbar^2/2ma^2)(n + \tfrac{1}{2})^2 f_{-(n+1)}. \qquad (18)$$

Thus, all eigenvalues, including the ground-state eigenvalue $\pi^2\hbar^2/8ma^2$, are *doubly degenerate*. We further see that although the Hamiltonian H, the parity operator P, and the time-reversal operator T commute, the two ground states f_0 and f_{-1} are *not* eigenstates of either the parity operator or the time-reversal operator.

$$(Tf_0)(x) = (Pf_0)(x) = f_{-1}(x), \qquad (19)$$

$$(Tf_{-1})(x) = (Pf_{-1})(x) = f_0(x). \qquad (20)$$

Thus, parity and time reversal are spontaneously broken symmetries.[3]

It is possible to restore these symmetries by defining states

$$g_n^+(x) = 2^{-1/2}[f_n(x) + f_{-(n+1)}(x)] = a^{-1/2}\cos(n + \tfrac{1}{2})\pi x/a, \qquad (21)$$

$$g_n^-(x) = 2^{-1/2} i[-f_n(x) + f_{-(n+1)}(x)] = a^{-1/2}\sin(n + \tfrac{1}{2})\pi x/a. \qquad (22)$$

These are now simultaneous eigenstates of H, P, and T:

$$(Pg_n^\pm)(x) = \pm g_n^\pm(x), \qquad (23)$$

$$(Tg_n^\pm)(x) = g_n^\pm(x), \qquad (24)$$

$$Hg_n^\pm = (\pi^2\hbar^2/2ma^2)(n + \tfrac{1}{2})^2 g_n^\pm. \qquad (25)$$

Thus, parity and time reversal are no longer broken symmetries. In this case, however, we have an even more surprising symmetry breaking, for although the momentum operator p and the Hamiltonian $p^2/2m$ commute, the eigenstates of the Hamiltonian are not eigenstates of the momentum operator. In fact,

$$pg_n^\pm = \mp(\pi\hbar/a)(n + \tfrac{1}{2})g_n^\mp, \qquad (26)$$

so that in particular,

$$pg_0^+ = -(\pi\hbar/2a)g_0^-, \qquad (27)$$

$$pg_0^- = (\pi\hbar/2a)g_0^+. \qquad (28)$$

In this case, we therefore have translational symmetry spontaneously broken since the translation operator,

$$U(\lambda) = e^{i\lambda p/\hbar}, \qquad (29)$$

does not leave the ground states $g_0^\pm$ invariant. In fact, by expanding

$$U(\lambda) = \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{i\lambda p}{\hbar}\right)^n, \qquad (30)$$

and repeatedly applying Eqs. (27) and (28) we get

$$U(\lambda)g_0^\pm = \cos(\pi\lambda/2a)g_0^\pm \mp i\sin(\pi\lambda/2a)g_0^\mp. \qquad (31)$$

This demonstrates conclusively that the translational symmetry is broken.

IV. INTERPRETATION OF THE MODEL

We now relate the mathematical model we have displayed to a definite physical system. If one considers a one-dimensional crystal consisting of only one type of atom, then the boundary condition in going from nearest neighbor to nearest neighbor is periodic. The situation repeats itself. Similarly, for a one-dimensional crystal with alternating atoms (*ABAB* . . .), as in an antiferromagnet, the boundary condition from an atom to its *next nearest* neighbor is periodic, and hence from nearest neighbor to nearest neighbor, antiperiodic.

We can now visualize the physical situation corresponding to our model and get a clearer understanding of the cause of the broken symmetry. If we consider such an antiferromagnetic crystal and consider the interval between nearest neighbors as fundamental, we must impose antiperiodic boundary conditions. Furthermore, since the endpoints correspond physically to different situations (atoms), it makes a difference whether a particle travels freely from left to right or right to left. The situations are not mirror images of each other, and hence, not eigenstates of the parity operator. Since time reversal reverses the direction of travel, these states are also not eigenstates of the time-reversal operator.

One can take a superposition of states of particles traveling to the left and right, as we did, to get standing waves which are then automatically time reversal as well as parity invariant. In this case, however, conservation of probability brings about a loss of translation invariance. The total probability in the interval $-a \leq x \leq a$ must be conserved as we translate the wave functions either to the left or right. Thus, whatever disappears beyond one endpoint, must reappear from the other endpoint as given by Eq. (31). Thus, the statement that $U(\lambda)$ is unitary (conserves probability), is the reason that these standing waves are not translation invariant. It is clear now that this "unusual" self-adjoint extension of the momentum operator has just as physical an interpretation as the usual one with periodic boundary conditions.

V. CONCLUSION

The example given is rather simple, yet it illustrates that by choosing periodic boundary conditions one has eliminated the physically interesting case of broken symmetries. The point is that if there are several self-adjoint extensions possible, only physics, not mathematics, can dictate which to choose. Thus, in such cases it is not mere pedantry to examine what the possible self-adjoint extensions are.

With respect to the model presented, it also illustrates many of the important points of models with spontaneously broken symmetry[3]: (1) The ground state is degenerate and is not invariant under a symmetry of the Hamiltonian; and

(2) In the second case, where translational symmetry is broken, the generator of this symmetry, namely p, is given by a representation which is unitarily inequivalent to the standard (periodic boundary conditions) representation for which the ground state is unique.

There is, however, no Goldstone mode[3] in either case, as can easily be checked by computing the Green's function which has no zero-energy pole.

It is, perhaps, also worthwhile to notice that the commutation relation

$$[x,p] = i\hbar, \tag{32}$$

is not valid in this representation, since for f in the domain of the momentum operator p, xf is not in the domain of p in general. In fact, in this case xf is in the domain of p only if $f(a) = f(-a) = 0$. Nevertheless, it is still true that

$$[x^{2n},p] = 2n\, i\hbar x^{2n-1}, \qquad n = 0,1,2,\ldots. \tag{33}$$

The identical situation occurs for the momentum operator defined with periodic boundary conditions. This is merely a reflection of the fact that p is defined over a finite interval.[4]

ACKNOWLEDGMENT

I have benefited from conversations with Dr. H. J. Kreuzer and Dr. M. Razavy. Work supported in part by the National Research Council of Canada.

[1]To see this, one need only examine any one of the standard textbooks on quantum mechanics. A very physical introduction to self-adjointness, together with definitions of hermitian and self-adjoint, is presented by A. S. Wightman, in *Cargèse Lectures in Theoretical Physics*, edited by M. Levy (Gordon and Breach, New York, 1964), pp. 262–268.

[2]In the case of angular momentum, the choice $\alpha = \frac{1}{2}$ was discussed by E. Merzbacher, Am. J. Phys. **30**, 237 (1962).

[3]Several elementary models of spontaneously broken symmetry are to be found in W. S. Hellman and P. Roman, Am. J. Phys. **35**, 614 (1967).

[4]The best known of these examples is the commutation relation between L_z and ϕ. This case is discussed in some detail in P. Carruthers and M. M. Nieto, Rev. Mod. Phys. **40**, 411 (1968).

PERPLEXITIES OF QUANTUM PHYSICS

Every other great idea of physics we know how to summarize in a few simple words, but not the quantum. To many even today the quantum idea comes as if strange and unwelcome and, as it were, forced upon one from the outside against one's will. In contrast if one really understood the central point and its necessity in the construction of the world one ought to be able to state it in one clear, simple sentence. Until we see the quantum principle with this simplicity we can well believe that we do not know the first thing about the universe, about ourselves, and about our place in the universe.

–John Archibald Wheeler