Origin of the anomalies: The modified Heisenberg equation

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The origin of the anomalies is analyzed. It is shown that they are due to the fact that the generators of the symmetry do not leave the domain of definition of the Hamiltonian invariant and thus a term, normally forgotten in the Heisenberg equation, gives an extra contribution responsible for the nonconservation of the charges. This explanation is equivalent to that of Fujikawa in the path integral formalism. Finally, this approach is applied to conformal symmetry breaking in two-dimensional quantum mechanics.

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The use of the symmetries of a system is one of the most fruitful techniques in physics, especially for quantum systems. Among the consequences of symmetry in quantum physics are selection rules, relations between matrix elements of observables, degeneracies in energy, and especially the existence of conservation laws which are guaranteed by Noether's theorem or its equivalent, the Ehrenfest equation. In particular, the evolution of the expectation values of an operator B is given by the Heisenberg equation

$$\frac{d}{dt}\langle\Psi(t)|B\Psi(t)\rangle=\left\langle\Psi(t)\left|\frac{\partial B}{\partial t}\Psi(t)\right.\right\rangle + \frac{i}{\hbar}\langle\Psi(t)|[H,B]\Psi(t)\rangle, \tag{1}$$

which says that for any group of symmetry whose elements (or generators in the associated Lie algebra) commute with the Hamiltonian H, if such operators do not depend explicitly on time t, their expectation value in any physical state must be constant with t.

Even for the case when the symmetry is not exact (it is explicitly broken), the Heisenberg equation (1) shows how the expectation values of the corresponding generators evolve with time. This has been largely used, for example, in particle physics where the flavor symmetry is explicitly broken by mass terms, or in nuclear physics where isospin symmetry is broken by the Coulomb interaction between protons and by the up-down quark mass difference.

However, there are some cases where, although the symmetry is exact at the classical level, it is not preserved in the corresponding quantum theory. This is the anomalous symmetry breaking that was first discovered in quantum field theory when studying certain Feynman diagrams, and further in the analysis of $\pi^0\to 2\gamma$ decay [1], and also in the Schwinger model [2]. In the path integral formalism, the existence of anomalies can be viewed as a consequence of the fact that, in this case, even if the classical Lagrangian is invariant under the symmetry, the measure is not [3], which gives rise to extra surface terms that are the origin of the anomaly.

In the Hamiltonian formalism, the anomaly can be understood as a consequence of the fact that the Heisenberg equation (1) is exact only if the domain of definition of the Hamiltonian is invariant with respect to the operator B; in other cases, an extra term appears which is responsible for the anomaly [4]. To be more precise, let H be the quantum Hamiltonian, which is self-adjoint when defined on a domain D_H; then for any physical state in the Hilbert space $\mathcal{H}$ and any operator B we have

$$\frac{d}{dt}\langle\Psi(t)|B\Psi(t)\rangle = \left\langle\Psi(t)\left|\frac{\partial B}{\partial t}\Psi(t)\right.\right\rangle + \frac{i}{\hbar}[\langle H\Psi(t)|B\Psi(t)\rangle - \langle\Psi(t)|BH\Psi(t)\rangle]$$

which can be written as

$$\frac{d}{dt}\langle\Psi(t)|B\Psi(t)\rangle = \left\langle\Psi(t)\left|\frac{\partial B}{\partial t}\Psi(t)\right.\right\rangle + \frac{i}{\hbar}\langle\Psi(t)|[H,B]\Psi(t)\rangle+\mathcal{A}, \tag{2}$$

where the anomaly $\mathcal{A}$ is defined as

$$\mathcal{A}=\frac{i}{\hbar}\langle\Psi(t)|(H^+-H)B\Psi(t)\rangle, \tag{3}$$

and in Eq. (2) the commutator $[H,B]$ is defined in the whole Hilbert space. Equivalently, in the Heisenberg picture, we obtain that for any operator B the derivative with respect to the time obeys a generalized Heisenberg equation:

$$\frac{dB}{dt}=\frac{\partial B}{\partial t}+\frac{i}{\hbar}[H,B]+\frac{i}{\hbar}(H^+-H)B. \tag{4}$$

Comparing Eqs. (1) and (2) we see that the Heisenberg equation (1) is exact only whenever B keeps invariant the domain of definition D_H of the Hamiltonian, because if $B\Psi_h\in D_H$ for $\Psi_h\in D_H$, then the extra term $\langle\Psi_h(t)|(H^+-H)B\Psi_h(t)\rangle=0$ as long as $H^+=H$ when acting on states of D_H. But when B does not keep D_H invariant, that is, $B\Psi_h\notin D_H$, the extra term will give a surface contribution responsible for the anomaly. In general, it is said that in the presence of an anomaly, the commutator of the Hamiltonian with the corresponding charges has two contributions, the

regular one and an extra part originated by the anomaly, $[H,B]_{total}=[H,B]_{reg}+[H,B]_{anom}$. We see that the so-called regular part is nothing but the commutator of the extension of the operators to the whole Hilbert space and the anomalous term is just $(H^+-H)B$.

It is easy to prove that the above description of the anomalies is equivalent to that of the path integral [3]. For example, in quantum mechanics, the Feynman propagator is

$$K(z,t;y,0)=\int_{x(t)=z}^{x(0)=y}[d\mu(x)]\exp[iS(x,\dot{x})/\hbar]$$
$$=\sum\int_n \varphi_n^*(y)\varphi_n(z)e^{-(iE_nt/\hbar)}, \tag{5}$$

where φ_n are the eigenvectors of the Hamiltonian and $\Sigma_n\int$ means a sum over the discrete and an integral over the continuum spectrum. In this sense, different self-adjoint extensions $H^{(\lambda)}$ of the quantum Hamiltonian associated with the same classical Lagrangian give rise to different sets of orthonormal eigenvalues $\varphi_n^{(\lambda)}(x)$, depending on the self-adjoint extension defined on $D_H^{(\lambda)}$, and each of them is characterized by a different measure in the path integral version, so if a particular domain of definition $D_H^{(\lambda)}$ is not invariant under the operator B, the same is true for the associated measure. The proof for quantum field theories is equivalent.

It should be noted that the existence of an anomaly is independent of the need or not for a regularization process for the theory, as can be seen in some quantum mechanical systems such as that of a charged particle moving on a two-torus and coupled to an electromagnetic field (see [5] and also [6]).

Recently, there has been a renewed interest in anomalies in conformal quantum mechanics: the three-dimensional $1/r^2$ potential which is relevant as an example of an anomaly in molecular physics [7], and the two-dimensional δ interaction [8]. In what follows, we shall analyze the latter in the light of the generalized Heisenberg equation (2). The problem is that of a free particle in two-dimensional quantum mechanics with a $\delta^2(r)$ interaction:

$$H=\frac{P^2}{2m}+\lambda\frac{1}{r}\delta(r). \tag{6}$$

It can be seen that considering the extension of H to the whole Hilbert space $\mathcal{H}=L^2(R_+,rdr)\otimes L^2(S_1,d\varphi)$, the theory is scale invariant, that is, the dilation operator $D=tH-G$ [where $G=(1/4)(\mathbf{rp}+\mathbf{pr})$], the conformal generator $K=-t^2H+2tD+(1/2)r^2$, and H close on commutation:

$$\frac{i}{\hbar}[K,D]=K, \tag{7}$$

$$\frac{i}{\hbar}[H,K]=-2D, \tag{8}$$

$$\frac{i}{\hbar}[D,H]=H, \tag{9}$$

showing that the invariance algebra is SO(2,1). The above equations together with the classical Heisenberg equation (1) mean that $(d/dt)\langle K\rangle=(d/dt)\langle D\rangle=0$, and that there cannot be any normalizable bound state with energy different from 0. However, in order to properly define the quantum theory, we must first define the domain of definition D_H of the Hamiltonian in such a way that $\overline{D_H}=\mathcal{H}$, and so that when acting on D_H we have $H^+=H$. In order to do that, we start by removing the origin to avoid the singularities of the Hamiltonian, and then working on $\dot{\mathbf{R}}^2=\mathbf{R}^2/\{0,0\}$ [9] and in polar coordinates, so the Hamiltonian reads

$$H=-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}\right). \tag{10}$$

The first question is to define the domain of definition of the operator $d^2/d\varphi^2$. In order to do that we start by looking for normalizable solutions of the equations

$$\frac{d^2}{d\varphi^2}\xi_\pm(\varphi)=\pm i\xi_\pm(\varphi). \tag{11}$$

In this case, there are two linearly independent solutions $\xi_\pm^\alpha(\varphi)(\alpha=1,2)$ for each equation, so the deficiency indices are $d_+=d_-=2$, and there are infinitely many self-adjoint extensions associated with different physical situations. Here we shall start with the one with periodic boundary conditions. Defining $d^2/d\varphi^2$ on

$$d_0=\{f(\varphi)\in L^2(S_1,d\varphi)\,|\,f(0)=f(2\pi);f'(0)=f'(2\pi)\}, \tag{12}$$

in that case, acting on d_0 the eigenfunctions of $d^2/d\varphi^2$ are $\xi_n(\varphi)=(2\pi)^{-1/2}e^{in\varphi}$ with $n\in Z$, and then D_H can be written as the direct sum

$$D_H=\bigoplus_{n\in Z}[D_n(R_+,rdr)\otimes\xi_n(\varphi)], \tag{13}$$

where $D_n(R_+,rdr)$ must be chosen in such a way that the radial part of the Hamiltonian

$$H_r=-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}-\frac{n^2}{r^2}\right) \tag{14}$$

is self-adjoint. For $n\neq0$ the deficiency indices of H_r are (0,0) so it is essentially self-adjoint acting on functions which vanish at $r=0$ and infinity. But for $n=0$ the deficiency indices are (1,1) and there are infinitely many self-adjoint extensions characterized by a parameter β:

$$D_{n=0}^\beta=\left\{f(r)\in L^2(R_+,rdr)\,\middle|\,\lim_{r\to0}\left(\frac{f(r)}{\log(\alpha_0r)}\right)\right.$$
$$\left.=\beta\lim_{r\to0}\left[f(r)-\lim_{r'\to0}\left(\frac{f(r')}{\log(\alpha_0r')}\right)\log(\alpha_0r)\right]\right\}, \tag{15}$$

where $\alpha_0^2=(2m\Lambda_0/\hbar^2)$, and Λ_0 is the dimensional constant we must introduce in order to make the deficiency index equations $H_r\Psi_\pm(r)=\pm i\Lambda_0\Psi_\pm(r)$ dimensionally consistent. The case $\beta=0$ is Friedrich's extension and corresponds to the situation $\lambda=0$ in (6), whereas $\beta\neq 0$ accounts for the case $\lambda\neq 0$.

Equation (15) means that if $f(r)\in D^\beta_{n=0}$ then for $r\to 0$, $f(r)\sim a[\log(\alpha r)+b]+O(r)$ with

$$\frac{1}{\beta}=b+\log\left(\frac{\alpha}{\alpha_0}\right). \tag{16}$$

Now, it can be seen that for $n\neq 0$ we have $GD_n\subset D_n$ so G leaves $D_{n\neq 0}$ invariant, but for $n=0$, $\beta\neq 0$, and $f(r)\in D_0^\beta$, we obtain that for $r\to 0$

$$\begin{aligned} f(r)&\sim a\left(\log(\alpha_0 r)+\frac{1}{\beta}\right)+O(r),\\ Gf(r)&\sim a\left(\log(\alpha_0 r)+\frac{1}{\beta}+1\right)+O(r), \end{aligned} \tag{17}$$

and consequently

$$G\,f(r)\in D_0^{\beta'},\quad \beta'=\frac{\beta}{\beta+1}, \tag{18}$$

so D_0^β is not invariant under the action of G, and consequently it is not invariant with respect to D and K. Hence the symmetry will be anomalously broken. The most relevant manifestation of this anomalous symmetry breakdown is the existence of a normalizable bound state

$$\Psi_0(r,\varphi)=\frac{\alpha}{\pi^{1/2}}K_0(\alpha r) \tag{19}$$

with energy

$$E_0=-\frac{\hbar^2}{2m}\alpha^2, \tag{20}$$

where if $\Psi_0\in D_0^\beta$ then α and β are related by $1/\beta=\log(\alpha/2\alpha_0)+\gamma$ (γ is Euler's constant). In this case for the dilation operator D the left side of Eq. (2) evaluates to E_0 whereas for the right side we have that $\langle\Psi_0|(\partial D/\partial t)\Psi_0\rangle=-(i/\hbar)\langle\Psi_0|[H,D]\Psi_0\rangle$, and Eq. (2) reduces to

$$\frac{d}{dt}\langle\Psi_0|D\Psi_0\rangle=\mathcal{A}=\frac{i}{\hbar}\langle\Psi_0|(H^+-H)D\Psi_0\rangle. \tag{21}$$

Integrating by parts, we finally obtain

$$\begin{aligned} \mathcal{A}=\frac{\hbar^2\alpha^2}{2m}\Bigg\{&\left[r\frac{d}{dr}K_0(\alpha r)\left(r\frac{d}{dr}+1\right)K_0(\alpha r)\right]_0^\infty\\ &-\left[rK_0(\alpha r)\frac{d}{dr}\left(r\frac{d}{dr}+1\right)K_0(\alpha r)\right]_0^\infty\Bigg\}=-\frac{\hbar^2\alpha^2}{2m}. \end{aligned} \tag{22}$$

Then we see that it is precisely the fact that D does not keep D_0^β invariant which causes the extra contribution that accounts for the value of the left side.

Finally, we can consider what happens with other self-adjoint extensions of the Hamiltonian. For example, defining the operator $d^2/d\varphi^2$ with vanishing boundary conditions on $d_v=\{f(\varphi)\in L^2(S_1,d\varphi)|f(0)=f(2\pi)=0\}$, everything, respective to the anomaly, is equivalent to the case of periodic boundary conditions, except that now $n=1,2,\ldots$ so there is not the $n=0$ sector; but if we define $d^2/d\varphi^2$ on

$$\begin{aligned} d_\theta=\{&f(\varphi)\in L^2(S_1,d\varphi)|f(0)\\ &=e^{i2\pi\theta}f(2\pi),\\ &f'(0)=e^{i2\pi\theta}f'(2\pi);\theta\in[0,1)\} \end{aligned} \tag{23}$$

then the domain of definition of H can be written as $D_H=\oplus_{n\in Z}[D_{n,\theta}(R_+,rdr)\otimes(2\pi)^{-(1/2)}e^{i(n+\theta)\varphi}]$, and for $\theta\neq 0$ the deficiency indices of the radial part of the Hamiltonian

$$H_r^\theta=-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}-\frac{(n+\theta)^2}{r^2}\right) \tag{24}$$

are $(0,0)$ for $n\neq 0,-1$, and $(1,1)$ for $n=0,-1$. In this last case, defining the adequate domains $D_{0,\theta}^\beta$ and $D_{-1,\theta}^{\beta'}$ it is easy to see that both subspaces are not invariant under G, which results in the fact that there are two normalizable bound states.

In conclusion, it has been shown that the origin of the anomalous symmetry breakdown is that the generators of the symmetry do not leave invariant the domain of definition of the Hamiltonian and thus, although the formal commutator of those generators with H vanishes, the charges are not conserved due to the extra surface term that appears in the exact Heisenberg equation (2). For the case of conformal symmetry breaking in the $\delta^2(r)$ potential, the anomaly has been calculated exactly and Eq. (2) verified. Similar results for the $1/r^2$ potential in three-dimensional quantum mechanics will be discussed elsewhere.

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