Electronic Structure of Super Heavy Atoms. Revisited.

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Point-like nucleus (Coulomb field)

For an electron, Coulomb field of a nucleus Ze can be considered as external since $m_p/m_e \sim 2000$. E.g., for the uranium $E = 900E_c$, at $R = 1, 2A^{1/3}$ fm.

Usually, electron spectrum in Coulomb f. is identified with the Dirac operator spectrum,

$$\hat{H}\left(Z\right) = -i\hbar c\boldsymbol{\alpha}\boldsymbol{\nabla} + \beta mc^2 - \frac{Ze^2}{r} \ ,$$

which was given by Sommerfeld (1940). Here there exists so-called "$Z_c = \alpha^{-1} \simeq 137, 04$ **catastrophe**"! If $Za > j + 1/2$, the spectrum becomes imaginary. E.g., for the lowest level

$$E = mc^2\sqrt{1 - \left(Za\right)^2}.$$

Gordon (1928): **"no regular solutions for ground state are found beyond Z_c."** This is repeated in all articles and books, Akhiezer, Berestetskiĭ, 1969; Greiner, Müller, Rafelski, 1985. The reason: **point-like nucleus in calculating the spectrum.**

Nucleus of a finite radius

A nucleus of a finite size, cutoff at $R \sim 1,2 \times 10^{-12}$cm, the Dirac equation has physically reasonable solutions for $Z < 173$. But for $Z \geq 173$ another difficulty arises (Popov 1970,1971)
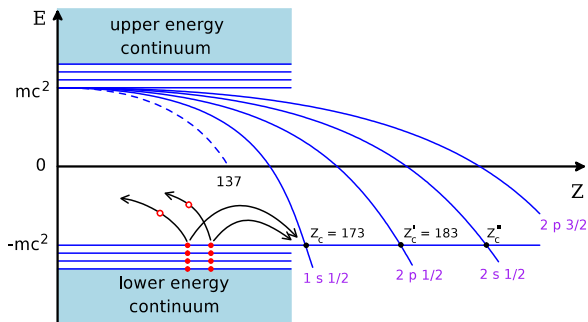
They believed that the problem can no longer be considered a one-particle one. There exists spontaneous pair production and screening of the Coulomb potential becomes essential.

Returning again to Coulomb field of point-like nucleus

Not disputing the fact that taking account of a finite size of the nucleus corresponds to a more realistic setting up the problem, we do not agree with the assertion that the Dirac Hamiltonian with the Coulomb field of overcritical point-like nucleus is inconsistent! **The difficulties with the spectrum for $Z > Z_c$ do not arise if the Dirac Hamiltonian is correctly defined as a self-adjoint (s.a.) operator!**

A rigorous treatment of this problem based on von Neumann theory of s.a. extensions of symmetric operators and Krein method of guiding functionals is presented in:

Gitman, Tyutin, Voronov, Theor.Math.Phys. 150 (2007) 34;
Self-adjoint Extensions in Quantum Mechanics (Birkhäuser 2012)

It was demonstrated that a definition of the Dirac Hamiltonian as a s.a. operator presents no problem for arbitrary Z.

Adjoint, self-adjoint, and symmetric operators

Consider a linear operator $\hat{f}$ and a linear equation for pairs of vectors ξ_*, η_*:

$$\left(\xi_*, \hat{f}\xi\right) = \left(\eta_*, \xi\right), \ \forall \xi \in D_f, \tag{1}$$

(**defining equation for adjoint operator** $\hat{f}^+$). ! η_* is uniquely determined by ξ_*: $\xi_* \xrightarrow{\hat{f}^+} \eta_*$, or $\eta_* = \hat{f}^+\xi_*$. Then $\hat{f}$ has **the adjoint operator** $\hat{f}^+$, its domain $D_{f^+} \in L^2(\mathbb{R})$ consists of such ξ_* for which there exist vectors η_* satisfying eq.(1).

$\hat{f}^+$ has to be calculated!

Self-adjoint $\hat{f}$: $\hat{f}^+ = \hat{f}$, in particular, $D_{f^+} = D_f$.

Compare: $\hat{f}$ is called **symmetric operator, or Hermitian operator**!, if

$$\left(\eta, \hat{f}\xi\right) = \left(\hat{f}\eta, \xi\right), \ \forall \xi, \eta \in D_f .$$

In the general case: **symmetric operator is not self-adjoint, but self-adjoint is always symmetric.**

S.a. Dirac Hamiltonians with the Coulomb field

A specific feature of the overcritical charges is a nonuniqueness of s.a. Dirac Hamiltonian, but this nonuniqueness is characteristic even for

$$Z > Z_{\mathrm{s}} = \left(\sqrt{3}/2\right)\alpha^{-1} \simeq 118, 68.$$

One can see that a s.a. Dirac Hamiltonian $\hat{H}(Z)$ with $Z \leq Z_{\mathrm{s}}$ is defined uniquely. For each $Z \geq Z_{\mathrm{s}}$, there exist a family $\{\hat{H}_{\nu_1,\ldots,\nu_\Delta}(Z)\}$ of s.a. Hamiltonians parametrized by a finite number of parameters

$$\nu_i \in [-\pi/2, \pi/2], \ -\pi/2 \sim \pi/2, \ i = 1,\ldots,\Delta = 2k(Z),$$
$$k(Z) = (1/4 + Z^2\alpha^2)^{1/2} - \delta, \ 0 < \delta \leq 1.$$

Any specific s.a. Dirac Hamiltonian $\hat{H}_{\nu_1,\ldots,\nu_\Delta}(Z)$ corresponds to a certain prescription for a behavior of an electron at the origin and specified by some boundary conditions for the wave function at the origin. A real spectrum and a complete set of eigenstates can be evaluated for each $\hat{H}_{\nu_1,\ldots,\nu_\Delta}(Z)$ with arbitrary Z.

S.a. Dirac Hamiltonians with Coulomb field

Dirac Hamiltonian $\hat{H}(Z)$ is a s.a. operator in the Hilbert space of s.-integrable bispinors $\Psi(\mathbf{r})$. On its domain $\hat{H}(Z)$ acts by the differential operation

$$\check{H}(Z) = \gamma^0 (\gamma \check{\mathbf{p}} + m) - qr^{-1}, \ \check{\mathbf{p}} = -i\boldsymbol{\nabla}, \ r = |\mathbf{r}|, \ q = Z\alpha.$$

Three commuting s.a. operators $\hat{\mathbf{J}}^2$, $\hat{J}_z$, $\hat{K}$, where $\hat{\mathbf{J}}$ total angular momentum, and $\hat{K}$ a spin operator (all commute with $\hat{H}(Z)$),

$$\hat{\mathbf{J}} = \hat{\mathbf{L}} + \boldsymbol{\Sigma}/2, \ \hat{\mathbf{L}} = [\mathbf{r} \times \hat{\mathbf{p}}], \ \hat{K} = \gamma^0 \left[1 + (\boldsymbol{\Sigma}\hat{\mathbf{L}})\right].$$

Any $\Psi(\mathbf{r})$ can be represented as $\Psi(\mathbf{r}) = \sum_{j,M,\zeta} \Psi_{j,M,\zeta}(\mathbf{r})$,

$$\Psi_{j,M,\zeta}(\mathbf{r}) = \frac{1}{r} \left(\begin{array}{c} \Omega_{j,M,\zeta}(\theta,\varphi)f(r) \\ i\Omega_{j,M,-\zeta}(\theta,\varphi)g(r) \end{array} \right),$$

$\Omega_{j,M,\zeta}$ spherical spinors, $f(r)$, $g(r)$-radial functions,

$$\hat{\mathbf{J}}^2\Psi = j(j+1)\Psi, \ \hat{J}_z\Psi = M\Psi, \ \hat{K}\Psi = -\zeta(j+1/2)\Psi,$$
$$j = 1/2, 3/2, ...; \ M = -j, -j+1, ..., j; \ \zeta = \pm 1.$$

S.a. radial Hamiltonians with Coulomb field

$$\hat{H}(Z)\Psi(\mathbf{r}) = E\Psi(\mathbf{r}) \rightarrow \hat{h}(Z,j,\zeta)F(r) = EF(r),$$
$$F = (f(r)\diagup g(r)) \in L^2(\mathbb{R}_+) \oplus L^2(\mathbb{R}_+),$$

where $\hat{h}(Z,j,\zeta)$ $-$ some s.a. radial Hamiltonians acting as

$$\check{h}(Z,j,\zeta) = -i\sigma_2 d_r + \zeta(j+1/2)r^{-1}\sigma_1 - qr^{-1} + m\sigma_3 \ .$$

Von Neumann theory of s.a. extensions of symmetric operators:

$$\check{h}(Z,j,\zeta) \rightarrow \hat{h}(Z,j,\zeta) - \text{all s.a. radial Hamiltonians with } D_{\hat{h}(Z,j,\zeta)}$$

Initial symmetric operators $\hat{h}_{\text{in}}(Z,j,\zeta)$,
$D_{\hat{h}_{\text{in}}(Z,j,\zeta)} = \mathcal{D}(\mathbb{R}_+) \oplus \mathcal{D}(\mathbb{R}_+)$, where $\mathcal{D}(\mathbb{R}_+)$ $-$ space of smooth functions $f(r)$ with a compact support. Then

$$D_{\hat{h}_{\text{in}}(z,j,\zeta)} \subseteq D_{\hat{h}(z,j,\zeta)} \subseteq D_{\hat{h}_{\text{in}}^+(z,j,\zeta)} = D^*_{\check{h}(Z,j,\zeta)},$$

$D^*_{\check{h}(Z,j,\zeta)}$ **natural domains**: $F, \check{h}(Z,j,\zeta)F \in \mathbb{L}^2(\mathbb{R}_+)$. Domains
$D^*_{\check{h}(Z,j,\zeta)}$ and their restrictions $D_{\hat{h}(Z,j,\zeta)}$ can be calculated.

S.a. radial Hamiltonians with Coulomb field

Constructing s.a. radial Hamiltonians $\hat{h}(Z, j, \zeta)$ essentially depends on Z and j.

There are two regions, **nonsingular** and **singular** ones, where the problem of s.a. extensions has principally different solutions. These regions are separated by the **singular curve** $Z = Z_s(j)$,
$$Z_s(j) = \sqrt{j(j+1)}\alpha^{-1} = 118, 7;\ 265;\ 405;\ 544;\ \dots .$$
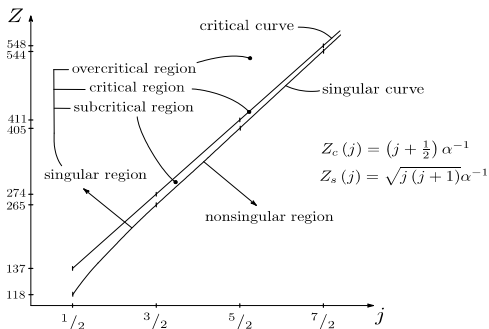
Nonsingular region

For $Z \leq Z_s(j)$ deficiency indices of each operator $\hat{h}_{in}(Z,j,\zeta)$ are zero and $\hat{h}(Z,j,\zeta) = \hat{h}_{in}^+(Z,j,\zeta)$ is a unique s.a. extension of $\hat{h}_{in}(Z,j,\zeta)$ with $D_{\hat{h}(Z,j,\zeta)} = D_{h(Z,j,\zeta)}^*(\mathbb{R}_+)$. Functions belonging to $D_{h(Z,j,\zeta)}^*(\mathbb{R}_+)$ have the following asymptotic behavior

$$F(r) = O(r^{1/2}), \ r \to 0; \ F(r) \to 0, \ r \to \infty.$$

A discrete spectrum $\{E_{n_\zeta}(Z,j,\zeta)\}$ of each $\hat{h}(Z,j,\zeta)$ has the form

$$E_{n_\zeta}(Z,j,\zeta) = \frac{m(n_\zeta + \gamma)}{\sqrt{q^2 + (n_\zeta + \gamma)^2}}, \ \gamma = \sqrt{(j+1/2)^2 - q^2},$$

$$n_1 = 1, 2, ...; \ n_{-1} = 0, 1, 2, ...; \ q = Z\alpha,$$

well-known Sommerfeld spectrum in the nonsingular region. This result justifies the standard formal treatment of the Dirac Hamiltonian with Z in the nonsingular region in the physical literature where the Hamiltonian is identified with the differential operation $\check{H}(Z)$ and the natural domain is implicitly assumed.

Singular region
General

In singular regions, $Z > Z_s(j)$, the deficiency indices of the operator $\hat{h}_{\mathrm{in}}(Z, j, \zeta)$ are $(1,1)$, there exists a family $\{\hat{h}_\nu(Z, j, \zeta)\}$ of its s.a. extensions, $\nu \in [-\pi/2, \pi/2]$, $-\pi/2 \sim \pi/2$.

At the same time, each $\hat{h}_\nu(Z, j, \zeta)$ is a nontrivial restriction of $\hat{h}_{\mathrm{in}}^+(Z, j, \zeta)$, such that $D_{\hat{h}_\nu(Z,j,\zeta)} \subset D_{h(q,\varkappa)}^*(\mathbb{R}_+)$.

Technically, it is convenient to divide the singular region into three subregions, we call them **subcritical, critical**, and **overcritical** regions.

The subregions are distinguished by a character of asymptotic boundary conditions at the origin specifying the domains $D_{\hat{h}_\nu(Z,j,\zeta)}$. The boundary conditions are similar in each subregion, which provides similar solutions of the corresponding spectral problems.

Subcritical region

$$\sqrt{j(j+1)}\alpha^{-1} = Z_s(j) < Z \leq Z_c(j) - \text{critical curve}$$

$$Z_c(j) = (j+1/2)\,\alpha^{-1} = 137;\ 274;\ 411;\ 548; \ldots .$$

S.a. Hamiltonians $\hat{h}_\nu(Z, j, \zeta)$ are specified by boundary conditions

$$F(r) = c[(mr)^\gamma d_+ \cos\nu + (mr)^{-\gamma} d_- \sin\nu] + O(r^{1/2}),\ r \to 0,$$

where $0 < \gamma = \sqrt{(j+1/2)^2 - q^2} < 1/2$, and $d_\pm$ some constant doublets.

The discrete spectrum consists of the points $\{E_{n_\zeta}^{(\nu)}(Z, j, \zeta)\}$ that obey the equation

$$\frac{\Gamma(1+2\gamma)\Gamma(-\gamma - qE\tau^{-1})[q(m-E) - (\varkappa + \gamma)\tau]}{\Gamma(\gamma - qE/\tau)[q(m-E) - (\varkappa - \gamma)\tau](2\tau/m)^{2\gamma}} = 0,$$

where $\varkappa = \zeta(j+1/2)$, $q = Z\alpha$, and $\tau = \sqrt{m^2 - E^2}$.

Subcritical region
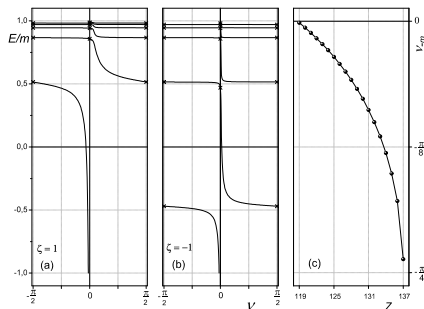
Figure: ν-dependence of energy levels $E_{n_\zeta}^{(\nu)}\left(121, 1/2, \zeta = \pm 1\right)$ and Z-dependence of ν_{-m}, $j = 1/2$.

The position of the discrete energy levels $E_{n_\zeta}^{(\nu)}\left(Z, j, \zeta\right)$ essentially depends on ν, in particular, there exists a value $\nu = \nu_{-m}$, for which the lower energy level coincides with the boundary $E = -m$ of the lower continuous spectrum.

Subcritical region

$E_{n_\zeta}^{(0)}(Z, j, \zeta)$ is the Sommerfeld spectrum. For $\nu = \pm\pi/2$, we have

$$E_{n_\zeta}^{(\pm\pi/2)}(Z, j, \zeta) = \frac{(n_\zeta - \gamma)m}{\sqrt{q^2 + (n_\zeta - \gamma)^2}} \ .$$

Critical region

The critical region is the critical curve $Z = Z_c(j)$. For integer Z, this region does not exist if the finite structure constant α is an irrational number, in particular, this region certainly is absent for $j = 1/2$.

S.a. radial Hamiltonians $\hat{h}_\nu(Z, j, \zeta)$ are specified by boundary conditions

$$F(r) = c\,[d_0(r)\cos\nu + d_+\sin\nu] + O(r^{1/2}\ln r),\ \ r \to 0,$$

where $d_0(r)$ are some doublet with the asymptotic behavior $d_0(r) = O(\ln mr)$ as $r \to 0$.

Overcritical region

The overcritical region $Z > Z_c(j)$.
S.a. radial Hamiltonians $\hat{h}_\nu(Z, j, \zeta)$ are specified by boundary conditions

$$F(r) = c\left[e^{i\nu}(mr)^{i\sigma}\rho_+ + e^{-i\nu}(mr)^{-i\sigma}\rho_-\right] + O(r^{1/2}), \ r \to 0,$$

$q = Z\alpha$, $\sigma = \sqrt{q^2 - (j + 1/2)^2} > 0$, and $\rho_\pm$ some constant doublets.
The discrete spectrum consists of the points $\{E_{n_\zeta}^{(\nu)}(Z, j, \zeta)\}$ that obey the equation

$$\cos\left[\frac{1}{2i}\sum_{a=1}^{3}\left[\ln(B_a) - \ln(B_a^*)\right] + \sigma\ln\frac{2\tau}{m} - \nu\right] = 0,$$

$B_1 = -2i\sigma$, $B_2(E) = i\sigma - Eq\tau^{-1}$, $B_3(E) = \tau(j + 1/2 - i\zeta\sigma) - \zeta q(m - E)$.

Overcritical region
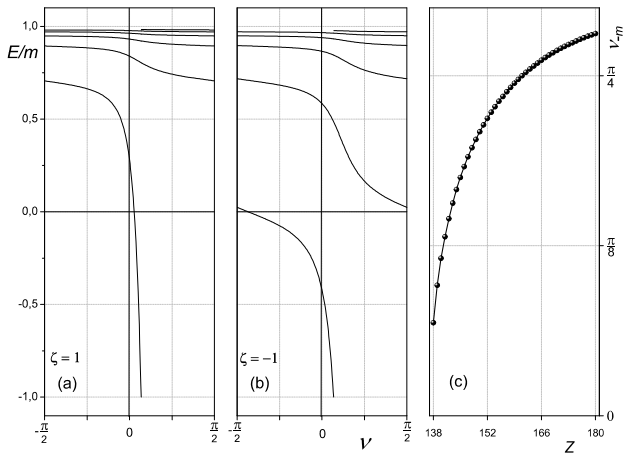
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Figure: ν-dependence of energy levels $E_{n_\zeta}^{(\nu)}$ $(180, 1/2, \zeta = \pm 1)$.

Concluding remarks
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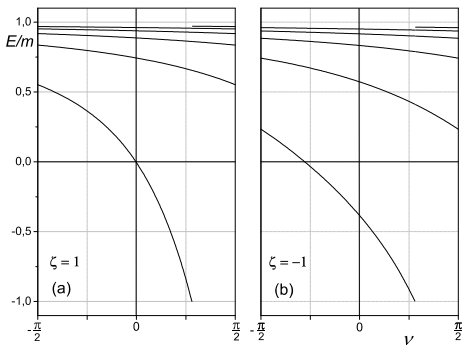- For any Z, the Dirac Hamiltonian $\hat{H}(Z)$ can be defined as a self-adjoint operator.
- For $Z \leq 118$ the Dirac Hamiltonian $\hat{H}(Z)$ is defined uniquely.
- For $Z \geq 119$, there exist family $\{\hat{H}_{\nu_1,...,\nu_\Delta}(Z)\}$ of possible total s.a. Dirac Hamiltonians. The family is parametrized by the parameters $\nu_i \in [-\pi/2, \pi/2]$, $-\pi/2 \sim \pi/2$, $i = 1, ..., \Delta$.

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- For any Z and any $\hat{H}_{\nu_1,\ldots,\nu_\Delta}(Z)$ spectra and inversion formulas are found. Eigenfunctions of the discrete spectrum and generalized eigenfunctions of the continuous spectrum form a complete orthonormalized system in $\mathbb{L}^2(\mathbb{R}_+)$.

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- For any Z and any $\hat{H}_{\nu_1,\ldots,\nu_\Delta}(Z)$ spectra and inversion formulas are found. Eigenfunctions of the discrete spectrum and generalized eigenfunctions of the continuous spectrum form a complete orthonormalized system in $\mathbb{L}^2(\mathbb{R}_+)$.
- The spectra of any s.a. Dirac Hamiltonian are simple (nondegenerate) and contain a continuous part occupying the two semiaxis $E \leq -m$ and $E \geq m$ and a discrete part $\{E_{n_\zeta}(Z, j, \zeta)\}$ located in the interval $|E| \leq m$.

Concluding remarks

- The discrete spectrum is always accumulated at $E = m$, and asymptotic form of the difference $E_{n_\zeta}(Z, j, \zeta) - m$ as $n_\zeta = n \to \infty$ is given by the well-known non-relativistic formula $E_n^{\text{nonrel}} = -mq^2 \left(2n^2\right)^{-1}$.

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- The position of discrete energy levels $E_{n_\zeta}^{(\nu)}(Z, j, \zeta)$ essentially depends on ν, in particular, for any $Z \geq 119$ there exists a value $\nu = \nu_{-m}$, for which the lower energy level coincides with the boundary $E = -m$ of the lower continuous spectrum, $E_0^{(\nu_{-m})}(Z, j, \zeta) = -m$. But

$$-m < E_{n_\zeta}^{(\nu)}(Z, j, \zeta) < m, \ \forall n \geq 0, \ \forall \nu \neq \nu_{-m} \ .$$

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- Generalizig Zeldovich-Popov interpretation for point-like nucleus: particle creation could start for $Z \geq 119$.

- Interesting coincidence: only nuclei with $Z \leq 118$ have been synthesised until now.

The end

Operators in Hilbert space. Adjoint operator

Hilbert space $\mathfrak{H} = L^2(a, b)$. A linear operator $\hat{f}$ with a domain $D_f \subseteq \mathfrak{H}$ is a linear mapping $D_f \longrightarrow \mathfrak{H}$. In general, D_f is not a *closed subspace*, $D_f \neq \overline{D_f}$; it is typical for unbounded operators, and is a specific feature of an infinite-dim. $\mathfrak{H}$. $\hat{f}$ is called **densely defined operator** *(DDO)*, if $\overline{D_f} = \mathfrak{H}$, it is typical for QM observables.

There is a stable distinction between the physical and mathematical terminologies at this point.

Let $\hat{p} = -i\hbar d_x$ in $L^2(\mathbb{R})$ (momentum operator for a one-dim. particle). In physical textbooks, $\psi_p(x) = \exp(ipx/\hbar)$ satisfying the differential equation $-i\hbar\psi_p'(x) = p\psi_p(x)$ is called the eigenfunction of $\hat{p}$ corresponding to the eigenvalue p.

But $\psi_p(x) \notin L^2(\mathbb{R})$, it is not s.-integrable on $\mathbb{R}$. Therefore, $\psi_p(x)$ is not an eigenfunction of $\hat{p}$, and p is not its eigenvalue; this function is the so-called generalized eigenfunction of $\hat{p}$, however, p is a point of the spectrum of $\hat{p}$ from the standpoint of a strict math. definition.

Adjoint, self-adjoint, and symmetric operators

Consider DDO $\hat{f}$ and a linear equation for pairs of vectors ξ_*, η_*:

$$\left(\xi_*, \hat{f}\xi\right) = (\eta_*, \xi)\,, \ \forall \xi \in D_f, \tag{2}$$

(**defining equation for adjoint operator** $\hat{f}^+$). $\quad$! $\ \eta_*$ is uniquely determined by ξ_*: $\xi_* \xrightarrow{\hat{f}^+} \eta_*$, or $\eta_* = \hat{f}^+\xi_*$. Then $\hat{f}$ has **the adjoint operator** $\hat{f}^+$, its domain $D_{f^+} \in L^2(\mathbb{R})$ consists of such ξ_* for which there exist vectors η_* satisfying eq.(2).
Self-adjoint DDO $\hat{f}$: $\hat{f}^+ = \hat{f}$, in particular, $D_{f^+} = D_f$.
Compare: A DDO $\hat{f}$ is called **symmetric operator, or Hermitian operator**!, if $\hat{f}^+$ is an extension of $\hat{f}$, $\hat{f} \subseteq \hat{f}^+$, i.e.,

$$\left(\eta, \hat{f}\xi\right) = \left(\hat{f}\eta, \xi\right)\,, \ \forall \xi\,, \eta \in D_f\,.$$

In the general case: **symmetric operator is not self-adjoint, but self-adjoint is always symmetric.**

In some textbooks on QM for physicists, this definition is considered the definition of a s.a. operator. This implicitly means that only bounded operators defined everywhere are considered. For unbounded operators, symmetricity and self-adjointness are different notions: self-adjointness implies symmetricity, but not vice versa. Symmetricity is generally insufficient for QM observables, they must be s.a..

If a symmetric operator $\hat{f}$ allows a symmetric extension $\hat{g}$, $\hat{f} \subseteq \hat{g}$, with $\hat{g} \subseteq \hat{g}^+$, then the chain of inclusions

We consider a very simple quantum-mechanical (QM) system: a free one-dimensional particle on an interval (a, b) and we shall see that by following the naive (extracted from simple textbooks on QM) precriptions literally, we arrive at certain paradoxes.

The phase space of this system is a strip, $(a, b) \times \mathbb{R}$, the position $x \in (a, b)$ and the momentum $p \in \mathbb{R}$. The evolution is defined by the Hamilton $\mathcal{H} = p^2/2m$. If $|a| < \infty$ and/or $|b| < \infty$, the peculiarity of this system is that its phase space is a space with boundaries.

The QM particle is assigned the position operator $\hat{x}$ and the

It is natural to take the x-representation of the commutation relations preserving the spectrum of $\hat{x}$ in the form $\mathrm{spec}\hat{x} = \{x \in (a, b)\}$, and, correspondingly, to realize the Hilbert space $\mathfrak{H} = L^2(a, b)$ of functions on (a, b), being square-integrable on this interval. Then $\hat{x}$ is the operator of multiplication by x:

$$\hat{x}\psi(x) = x\psi(x) , \qquad (4)$$

while $\hat{p}$ is:

$$\hat{p} = -i\hbar d_x : \ \hat{p}\psi(x) = -i\hbar\psi'(x) . \qquad (5)$$

The quantum Hamiltonian is:

$$\widehat{\mathcal{H}} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}d_x^2 . \qquad (6)$$

The position operator $\hat{x}$ seams to be a bounded, self-adjoint operator, $\hat{x} = \hat{x}^+$. Considering $\hat{p}$ as a self-adjoint operator, we have a set of three a self-adjoint operators $\hat{x}$, $\hat{p}$, and $\widehat{\mathcal{H}}$ with the commutation relations

$$[\hat{x}, \hat{p}] = i\hbar , \ \left[\hat{p}, \widehat{\mathcal{H}}\right] = 0 , \qquad (7)$$

Let $\psi_p(x)$ be an eigenvector of the momentum operator,
$\hat{p}\psi_p = p\psi_p$. Then

$$
\begin{aligned}
\left(\psi_p, [\hat{x}, \hat{p}]\psi_p\right) &= \left(\psi_p, \hat{x}\hat{p}\psi_p\right) - \left(\psi_p, \hat{p}\hat{x}\psi_p\right) \\
&= \left(\psi_p, \hat{x}\hat{p}\psi_p\right) - \left(\hat{p}\psi_p, \hat{x}\psi_p\right) \\
&= p[\left(\psi_p, \hat{x}\psi_p\right) - \left(\hat{x}\psi_p, \psi_p\right)] = 0,
\end{aligned} \tag{8}
$$

which is based on the self-adjointness of $\hat{p}$. It is clear that the
result (8) is in contradiction with a nonzero value of the
commutator $[\hat{x}, \hat{p}] = i\hbar$.

In addition, the latter commutator implies the Heisenberg
uncertainty relation

$$
\Delta x \Delta p \geq \frac{\hbar}{2}, \tag{9}
$$

where Δx and Δp are the respective dispersions of the position and
momentum. We recall that

$$
\Delta f = \sqrt{\langle (\hat{f} - \langle \hat{f}\rangle_\psi)^2 \rangle_\psi} = \sqrt{\langle \hat{f}^2\rangle_\psi - \langle \hat{f}\rangle_\psi^2}. \tag{10}
$$

Let us consider a particle in an infinite rectangular potential well (on the interval $[0, l]$). The eigenvalues and the eigenfunctions of the Hamiltonian in the case under consideration are well-known from any textbook:

$$\widehat{\mathcal{H}}\psi_n(x) = E_n\psi_n(x), \quad E_n = \frac{\hbar^2}{2m}\left(\frac{\pi}{l}\right)^2 n^2, \quad (11)$$

$$\psi_n(x) = \sqrt{\frac{2}{l}}\sin\left(\frac{\pi n}{l}x\right), \; n = 1, 2, \dots. \quad (12)$$

It is also well-known that the sequence $\psi_n(x)$ of these eigenfunctions is an orthobasis in $L^2(0, l)$, which confirms the self-adjointness of the Hamiltonian. It is know that any two commuting s.a. operators have common eigenvectors. In particular, if the spectrum of one of the commuting s.a. operators is nondegenerate then its eigenvectors must be eigenvectors of another s.a. operator. Here, we have two s.a. operators $\hat{p}$ and $\widehat{\mathcal{H}}$ commuting among themselves; moreover, the spectrum (11) of $\widehat{\mathcal{H}}$ is nondegenerate. Therefore, eigenfunctions (12) must be the eigenfunctions of $\hat{p}$; however,

In standard text-books on QM for physicists, it is believed that the matrix $f_{mn} = (e_m, \hat{f} e_n)$ of an operator $\hat{f}$ with respect to an orthobasis e_n completely defines the operator $\hat{f}$ by means of

$$\psi = \sum_{n=1}^{\infty} \psi_n e_n \, , \ \psi_n = (e_n, \psi) \, ,$$

$$\hat{f} e_n = \sum_{m=1}^{\infty} f_{mn} e_m \, ,$$

$$\hat{f} \psi = \sum_{m=1}^{\infty} \left(\sum_{n=1}^{\infty} f_{mn} \psi_n \right) e_m \, .$$

For example, the adjoint $\hat{f}^+$ of $\hat{f}$ is defined as an operator whose matrix elements are

$$\left(f^+ \right)_{mn} = \left(e_m, \hat{f}^+ e_n \right) = \left(\hat{f} e_m, e_n \right) = \overline{f_{nm}} \, .$$

Correspondingly, a self-adjoint operator, $\hat{f} = \hat{f}^+$, is defined as an operator whose matrix is Hermitian $f_{mn} = \overline{f_{nm}}$.

However, let us consider the set

$$e_n(x) = \sqrt{\frac{2}{l}} \cos\left(\frac{\pi n}{l} x\right) \ , \ n \in \mathbb{Z}, \tag{13}$$

which is complete in $L^2(0, l)$. Calculating the matrix elements $p_{mn} = (e_m, \hat{p}e_n)$ of the momentum operator $\hat{p}$ with respect to this set, we obtain

$$\overline{p_{nm}} = p_{mn} + i[e_m(l)e_n(l) - e_m(0)e_n(0)]$$
$$\neq p_{mn}, \tag{14}$$

so that the matrix p_{mn} is not Hermitian, contrary to our expectations.

Let us consider a state of a free particle in an infinite rectangular potential well (on a segment $[0, l]$ with the wave function

$$\psi(x) = Nx(x - l), \qquad (15)$$

and let us then calculate the mean value of the squared energy $\langle E^2 \rangle$ for such a state. On the one hand, due to the property $\left(\widehat{\mathcal{H}}\right)^2 \psi = 0$, this mean value must be zero:

$$\langle E^2 \rangle = \left(\psi, \left(\widehat{\mathcal{H}}\right)^2 \psi\right) = 0.$$

On the other hand, due to the self-adjointness of $\widehat{\mathcal{H}}$, we obtain a nonzero result for the same quantity:

$$\langle E^2 \rangle = \left(\widehat{\mathcal{H}}\psi, \widehat{\mathcal{H}}\psi\right) = \frac{N^2 \hbar^4 l}{m^2}.$$

Consider the Schrödinger equation

$$i\hbar\frac{\partial\psi\left(x,t\right)}{\partial t}=\widehat{\mathcal{H}}\psi\left(x,t\right) \qquad (16)$$

for a particle in an infinite rectangular potential well (on the segment $[0,l]$).

We recall that in the idealized quantization scheme the time-evolution problem in the form (16) can be posed for arbitrary initial states. Let us examine an initial (at $t=0$) state

$$\psi\left(x\right)=C\exp\left(\frac{i+1}{\sqrt{2}}\frac{kx}{\hbar}\right), \qquad (17)$$

where k is a certain fixed real parameter. The case of the initial state (17) is quite surprising, because it is easy to verify that the solution $\psi\left(t,x\right)$ of eq. (16) with the initial condition (17) is given by

$$\psi\left(t,x\right)=e^{-\frac{k^{2}}{2m\hbar}t}\psi\left(x\right). \qquad (18)$$

The evolution is not unitary; the wave function $\psi\left(t,x\right)$ "vanishes" with time. Of course, the reason is that

We recall that the first paradox is a consequence on the relation

$$\left(\psi_p, [\hat{x}, \hat{p}]\psi_p\right) = \left(\psi_p, \hat{x}\hat{p}\psi_p\right) - \left(\psi_p, \hat{p}\hat{x}\psi_p\right) = 0, \qquad (19)$$

Obviously, the uncertainty principle and canonical commutation relations are necessarily violated if (19) holds.

Consider a particle on the whole real axis $\mathbb{R}$ with the Hilbert space $L^2(\mathbb{R})$. Here there exists a unique self-adjoint momentum operator which acts as $-i\hbar d/dx$ on their domains of definition. However, such an operator has no eigenfunctions in $L^2(\mathbb{R})$, such that ψ_p in (19) do not exist.

Consider a particle on a semiaxis $\mathbb{R}_+$ with the Hilbert space $L^2(\mathbb{R}_+)$. Here there are no self-adjoint momentum operators at all, and therefore, eigenfunctions ψ_p in (19) do not exist.

Thus, no one quantity in (19) does not exist in the above two cases.

Applying von Neumann theory of self-adjoint extensions [1] to the case of momentum operator on the interval, one can find that there exists a one-parameter family of self-adjoint operators $\hat{p}_\vartheta$ with act as $-i\hbar d/dx$ on their domains of definition D_ϑ. The function

The eigenfunctions $\psi_{\vartheta n}(x)$, $n \in \mathbb{Z}$, of the operator $\hat{p}_{\vartheta}$ are

$$\hat{p}_{\vartheta}\psi_{\vartheta n} = p_{\vartheta n}\psi_{\vartheta n}, \quad \psi_{\vartheta n} = N \exp\left(i\frac{p_{\vartheta n}}{\hbar}x\right),$$

$$p_{\vartheta n} = \hbar\left(\frac{2\pi n + \theta}{l}\right) .$$

A solution of the first above mentioned paradox is related to the fact that the function $x\psi_{\vartheta}(x)$ does not belong to the domain of definition of the operator $\hat{p}_{\vartheta}$ (they do not obey (20)), such that the commutator $[\hat{x}, \hat{p}_{\theta}]$ is not defined on such a domain.

Since the Heisenberg uncertainty relation is derived considering matrix elements of the operator $[\hat{x}, \hat{p}]$, similar consideration allows one to explain the second part of the first paradox, related to the Heisenberg uncertainty relation.

We recall that the second paradox is a consequence of the supposition that the Hamiltonian of a free particle in an infinite rectangular potential well can be represented as $\widehat{\mathcal{H}} = \hat{p}^2/2m$, and, therefore it commutes with a s.a. momentum operator $\hat{p}$. Then both operators must have a common set of eigenfunctions, which is not true.

One can demonstrate that there exists only one s.a. Hamiltonian $\widehat{\mathcal{H}}$ of a particle in an infinite rectangular potential well. In particular, functions from the definition domain of $\widehat{\mathcal{H}}$ obey the condition

$$\psi(0) = \psi(l) = 0.$$

As was already said, on the finite interval all s.a. momentum operators are reduced to a family $\hat{p}_\vartheta$. Non of these operators allows the representation $\widehat{\mathcal{H}} = (\hat{p}_\vartheta)^2/2m$. Moreover, eigenfunctions of any $\hat{p}_\vartheta$ do not belong to the definition domain of $\widehat{\mathcal{H}}$. In fact, the operators $\widehat{\mathcal{H}}$ and $\hat{p}_\vartheta$ do not commute among themselves and have no common eigenfunctions (this is consistent with the physical fact that the particle momentum changes due to a reflection from the wall).

The third paradox treats matrix elements $p_{mn} = (e_m, \hat{p}e_n)$ of the operator $\hat{p}$ of a particle on an interval $[0, l]$, calculated with respect to the complete orthobasis e_n (13). It turns out that the matrix p_{mn} is not Hermitian, contrary to naive expectations. The incorrect supposition underlying the paradox is that the basis (13) belongs to the definition domain of a s.a. momentum operator of a particle on a finite interval $[0, l]$. However, we already know that there exists a family of s.a. momentum operators $\hat{p}_\vartheta$, with a definition domains D_{p_ϑ}. In particular, functions from D_{p_ϑ} must obey the condition (20). However,

$$e_n(l) = (-1)^n e_n(0). \tag{21}$$

Therefore, does not exist an angle ϑ, one and the same for all n, such that (21) could be identified with (20). I.e., does not exist a domain D_{p_ϑ} such that the complete basis e_n belongs to D_{p_ϑ}, or for any ϑ some elements of the basis e_n do not belong to definition domain of a s.a. operator $\hat{p}_\vartheta$, such that both quantities in inequality (14) do not exist, and, therefore, it has no sence.

The fourth paradox treats the case of a free particle in an infinite rectangular potential well on the interval $[0, l]$, with a s.a. Hamiltonian $\widehat{\mathcal{H}}$, for which

$$\left(\psi, \left(\widehat{\mathcal{H}} \right)^2 \psi \right) \neq \left(\widehat{\mathcal{H}} \psi, \widehat{\mathcal{H}} \psi \right) \tag{22}$$

in a particular state $\psi(x) = Nx(x - l)$ (15), where N is a normalization factor. An explanation of this paradox is the following: As it is known, there exists one s.a. Hamiltonian $\widehat{\mathcal{H}}$ of a particle in an infinite rectangular potential well. Functions from the definition domain obey the relation $\psi(0) = \psi(l) = 0$. One can see that the state (15) belongs to the domain of the Hamiltonian. However, the state $\widehat{\mathcal{H}}\psi = \text{const}$ already does not belong to the domain and, therefore, inequality (22) has no sence.

EXPLANATION OF THE FIFTH
PARADOX

In the last paradox, one consideres a solution of the Schrödinger equation for a free particle on the interval with a special choice (17) of the initial state and discoveres that such a solution vanishes with time, which means that the evolution is not unitary. As was aready mentioned this happens since the initial state does not belong to definition domain of any s.a. Hamiltonian on the interval, such that the left hand side of the Schrödinger equation is not defined.

Considering this paradox, we met a function that is a solution of the Schrödinger equation with a given initial date but with a nonunitary evolution. In this respect, we ought to note that in QM we have, in fact, two ways to define the time evolution: the first one is to solve the Cauchy problem for the Schrödinger equation with a given initial data and another one is to apply the unitary evolution operator $\hat{U}(t)$,

$$\hat{U}(t) = \exp\{-\frac{i}{\hbar}\hat{H}t\},$$

1.60217733 × 10^{-19} C
9.1093897 × 10^{-31} kg
2.99792458 × 10^8 m s^{-1}
6.6260755 × 10^{-34} J s

$$T \ll \pi\sqrt{\frac{\hbar}{2ce\alpha E}}\exp\left(\pi\frac{E_{\mathrm{c}}}{2E}\right),$$

$$E_{\mathrm{c}} = \frac{m^2 c^3}{e\hbar} \approx 1,3 \cdot 10^{16}\mathrm{V/cm} \ , \ \alpha = e^2/\hbar c.$$

for $E = E_c$, we have

$$T \ll \pi\sqrt{\frac{\hbar^2 137}{2m^2 c^4}}\exp\left(\frac{\pi}{2}\right) = \frac{\hbar\pi}{mc^2\sqrt{2}}\exp\left(\frac{\pi}{2}\right) = T_0\frac{\pi}{\sqrt{2}}\exp\left(\frac{\pi}{2}\right), \ T_0 \simeq$$