GENERALIZED DYNAMICAL THEORIES IN PHASE SPACE AND THE HYDROGEN ATOM

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GPTs with position and momentum

$\vec{q}, \vec{p} \in \mathbb{R}^3$ - position and momentum
$\rho(\vec{q}, \vec{p})$ - state is pseudo-probability density, $\iint_{\mathbb{R}^6} \rho(\vec{q}, \vec{p})\, \mathrm{d}^3q\mathrm{d}^3p = 1$
probability of observing position from interval I:

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The problem

Probability of observing energy from interval I: $\mathbb{P}_\rho(\tilde{H} \in I) = ???$

Phase space spectral measure

$g_A(I; \vec{q}, \vec{p})$ - phase space projector

$$\mathbb{P}_\rho(\tilde{A} \in I) = \int_{\mathbb{R}^2} g_A(I; \vec{q}, \vec{p}) \rho(\vec{q}, \vec{p}) \mathrm{d}^3 q \mathrm{d}^3 p$$

such that

$$g_A(\mathbb{R}; \vec{q}, \vec{p}) = 1, \qquad \int_{\mathbb{R}} a g_A(a; \vec{q}, \vec{p}) \, \mathrm{d}a = A(\vec{q}, \vec{p}).$$

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For discrete spectrum:

$$g_H(I; \vec{q}, \vec{p}) = \sum_{E_n \in I} g_H(E_n; \vec{q}, \vec{p})$$

such that

$$\sum_n g_H(E_n; \vec{q}, \vec{p}) = 1, \qquad \sum_n E_n g_H(E_n; \vec{q}, \vec{p}) = H(\vec{q}, \vec{p}).$$

Example: phase space spectral measures of position

$\chi(I; q_i)$ - characteristic function of interval

$$\mathbb{P}_\rho(\tilde{q}_i \in I) = \iint_{q_i \in I} \rho(\vec{q}, \vec{p}) \mathrm{d}^3 q \mathrm{d}^3 p = \iint_{\mathbb{R}^6} \chi(I; q_i) \rho(\vec{q}, \vec{p}) \mathrm{d}^3 q \mathrm{d}^3 p$$

We identify

$$g_{Q_i}(I; \vec{q}, \vec{p}) = \chi(I; q_i).$$

Generalized Moyal bracket

$$\dot{\rho} = \{\{H, \rho\}\}$$

$$\{\{f, g\}\} = \{f, g\} + \sum_{n=1}^{\infty} a_n \hbar^{2n} \left(f \{ \overleftarrow{\cdot}, \overrightarrow{\cdot} \}^{2n+1} g \right),$$

Time evolution

Generalized Moyal bracket

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Ehrenfest theorem

Time-evolution of mean values of q_i, p_j is classical.

Coefficient a_n are experimentally measurable

Implement $H(t) = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2 + \lambda(t) \frac{m^2\omega^3}{2\hbar} q^4$, measure p^2 at later time.

How to build a theory

1. For every observable define a function $A(\vec{q},\vec{p})$ such that $\langle\tilde{A}\rangle = \iint_{\mathbb{R}^6} A(\vec{q},\vec{p})\rho(\vec{q},\vec{p})\mathrm{d}^3q\mathrm{d}^3p$.
2. For every observable define the phase space spectral measure $g_A(I;\vec{q},\vec{p})$
3. Define the coefficients a_n of the generalized Moyal bracket $\{\{\cdot,\cdot\}\}$.
4. Define the set of states as the (convex subset of the) largest set of pseudo-probability distributions satisfying the **positivity conditions for states**:

$$\mathbb{P}_{\rho(t)}(\tilde{A}\in I) = \iint_{\mathbb{R}^6} g_A(I;\vec{q},\vec{p})\rho(\vec{q},\vec{p};t)\mathrm{d}^3q\mathrm{d}^3p \geq 0$$

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We always assume that position and momentum observables are:

$$Q_i(\vec{q},\vec{p}) = q_i \qquad g_{Q_i}(I;\vec{q},\vec{p}) = \chi(I;q_i)$$
$$P_i(\vec{q},\vec{p}) = p_i \qquad g_{P_i}(I;\vec{q},\vec{p}) = \chi(I;p_i)$$

TOY MODEL

Motivation from classical theory

Classical theory:

$$\mathbb{P}_\rho(\tilde{H} \in I) = \int_{E\in I} \int_{H(\vec{q},\vec{p})=E} \rho(\vec{q},\vec{p})\mathrm{d}^3q\mathrm{d}^3p \,\mathrm{d}E$$

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$\chi(I; H(\vec{q},\vec{p}))$ - piecewise constant function of $H(\vec{q},\vec{p})$.

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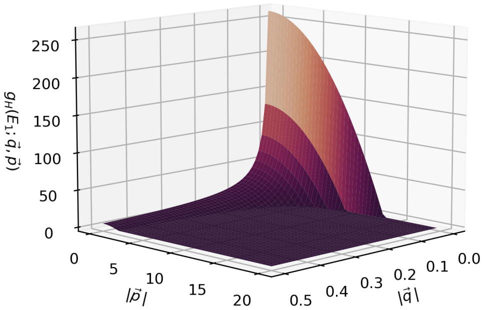
Main idea

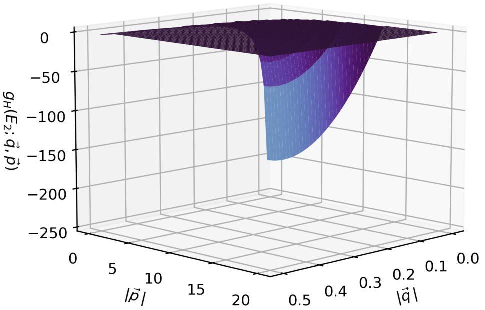
Take $g_H(I; \vec{q},\vec{p})$ - piecewise linear function of $H(\vec{q},\vec{p})$

Probabilities and the energy spectrum of the hydrogen atom

$H(\vec{q},\vec{p}) = \frac{|\vec{p}|^2}{2m} - \frac{\kappa}{|\vec{q}|}$.

There is **only one** set of piecewise linear functions $g_H(I;\vec{q},\vec{p})$ corresponding to the spectrum $E_n = E_1/n^2$ satisfying necessary and natural conditions.





Negativity of $g_H(E_2;\vec{q},\vec{p})$ implies position-momentum uncertainty and prevents collapse of the atom!

States of the hydrogen atom

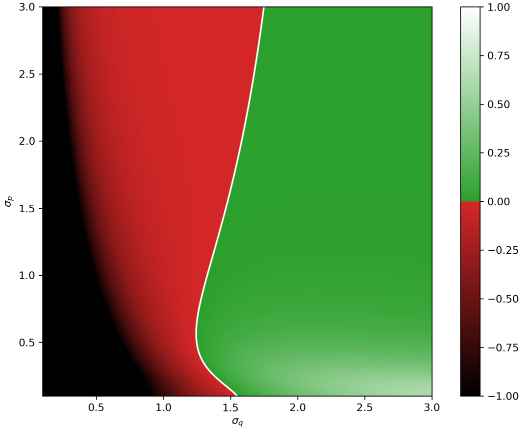
$$\rho_G(\vec{q},\vec{p}) = \frac{1}{(2\pi)^3\sigma_q^3\sigma_p^3}\,\mathrm{e}^{-\frac{|\vec{q}|^2}{2\sigma_q^2}-\frac{|\vec{p}|^2}{2\sigma_p^2}}$$

We have to enforce

$$\mathbb{P}_{\rho_G}(\tilde{H} = E_2) \geq 0.$$

Ground state

$$\rho_{\text{gnd}}(\vec{q},\vec{p}) = \frac{1}{(2\pi)^{\frac{3}{2}}\sigma_{\text{gnd}}^3}\,\mathrm{e}^{-\frac{|\vec{q}|^2}{2\sigma_{\text{gnd}}^2}}\,\delta^{(3)}(\vec{p})$$



External magnetic field

$H_B(\vec{q},\vec{p}) = H(\vec{q},\vec{p}) + \frac{\mu_B}{\hbar} B L_3(\vec{q},\vec{p})$

Take $g_{L_i}(I;\vec{q},\vec{p})$ - piecewise linear phase space spectral measure for angular momentum L_i. Construct

$$g_{H_B}(I) = \sum_{n,m:\ E_n + \mu_B B m \in I} g_H(n;\vec{q},\vec{p})\, g_{L_3}(m;\vec{q},\vec{p})$$

$g_{H_B}(I)$ - phase space spectral measure for the Hamiltonian $H_B(\vec{q},\vec{p})$.

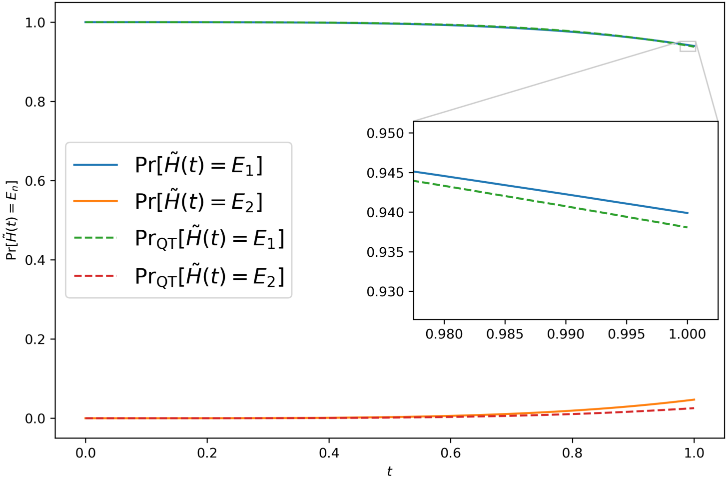
Result

Splitting of energy levels due to external magnetic field with

$$|m| < 2(n+1).$$

Perturbations by resonant light

$H_E(\vec{q}, \vec{p}, t) = H(\vec{q}, \vec{p}) - 2eE\sin(\omega t) q_3$, using interaction picture we get:



Scattering

Incoming particle density: $\rho_{\text{in}} = \nu\delta^{(3)}(\vec{p} - \vec{p}_0)$

Using Green's function approach we get:

$$\rho(t;\vec{q},\vec{p}) = \rho_{\text{in}}(t;\vec{q},\vec{p}) + \int\limits_{\mathbb{R}^3}\int\limits_{-\infty}^{t} K(\vec{q} - \frac{\vec{p}}{\mu}(t-\tau), \vec{p}, \vec{p'})\rho(\tau;\vec{q} - \frac{\vec{p}}{\mu}(t-\tau), \vec{p'})\,\mathrm{d}\tau\mathrm{d}^3p'$$

where

$$K(\vec{q},\vec{p},\vec{p'}) = \left\{\left\{ V(\vec{q}), \delta_p^{(3)}(\vec{p} - \vec{p'})\right\}\right\}.$$

Solved via $V(\vec{q}) \mapsto \lambda V(\vec{q})$ and comparing equal powers of λ.

Result

For $t \to \infty$ and $|\vec{q}| \to \infty$ we always get Rutherford formula $\frac{d\sigma}{d\Omega} = \frac{\kappa^2\mu^2}{4p_0^4}\frac{1}{\sin^4(\vartheta/2)}$

	Ehrenfest theorem	stable atom	quantized energy levels	Rutherford scattering	experimental predictions	Hilbert space formulation
CLASSICAL THEORY	✓	✗	✗	✓	✓	✓
QUANTUM THEORY	✓	✓	✓	✓	✓	✓
GENERALIZED WIGNER THEORY	✓	✓	✓	✓	✓	✗

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