

MAT 1723HF (APM 421H1F): MATHEMATICAL CONCEPTS OF QUANTUM MECHANICS AND QUANTUM INFORMATION

I. M. SIGAL TA: I. ANAPOLITANOS

1. COURSE ORGANIZATION

1.1. **Goals.** The goal of this course is to explain key concepts of Quantum Mechanics and to arrive quickly to some topics which are at the forefront of active research. Among the latter topics we cover Bose-Einstein condensation and quantum information. Both of these topics have witnessed an explosion of research in the last decade and both involve deep and beautiful mathematics.

1.2. **Mathematical rigour.** We will try to be as self-contained as possible and rigorous whenever the rigour is instructive. Whenever the rigorous treatment is prohibitively time-consuming we give an idea of the proof, if such exists, and/or explain the mathematics involved without providing all the details.

1.3. **Prerequisites.** For this course it is desirable to have some familiarity with elementary ordinary and partial differential equations. Knowledge of elementary theory of functions and operators would be helpful.

1.4. **Syllabus.** * Schrödinger equation

- * Quantum observables
- * Spectrum and evolution
- * Density matrix
- * Bose-Einstein condensation
- * Quasiclassical asymptotics
- * Approximate methods
- * Hartree-Fock theory
- * Open systems and Lindblad evolution
- * Quantum entropy
- * Quantum channels and information processing
- * Quantum Shannon theorems

1.5. **Break-up of material.** QM, Basic topics: [1], Chapters 1-5 and 7 (plus Resonances and Quasi-classics);

QM - Advanced topics: Hartree and Hartree-Fock approximations and BEC ([1], Section 8.9) and Open systems ([1], Sections 9.1-9.8);

Quantum information and quantum computations.

1.6. **Texts.** Textbook: S. Gustafson and I.M. Sigal: Mathematical Concepts of Quantum Mechanics, 2nd edition, Springer, 2005.

In covering information theory we will follow on-line material, papers and the books,

Michael A. Nielsen and Isaac L. Chuang, Quantum Computation and Quantum Information (Paperback - Sep 2000) Cambridge Univ Press, ISBN 0 521 63503 9 (paperback).

1.7. **Marking scheme.** Undergraduates:

Midterm test October 21-29 (take home).

Final test Dec 14, 2009, 2:00-5:00pm, Location: SS2127 (at least 2/3 of the problems are the same as in the midterm test, but 60% of the mark is due to the new problems).

Graduates: Above plus a 20 min presentation.

Breakup of the grade:

Undergraduates: 35%/65% (MT/F)

Graduates: 25%/35%/40% (MT/F/P)

1.8. **Schedule.** Thursdays, 3-6 pm, MP118 (McLennan Physics building).

1.9. **Webpage.** <http://www.math.utoronto.ca/ioanap/QMcoursesnotes.pdf>

REFERENCES

- [1] S. Gustafson and I.M. Sigal, *Mathematical Concepts of Quantum Mechanics*, 2nd edition, Springer, 2005
 [2] A. S. Holevo, *Statistical Structure of Quantum Theory*, Springer-Verlag (2001).
 [3] A. S. Holevo, *Probabilistic and Statistical Aspects of Quantum Theory*, Amsterdam, The Netherlands: North Holland.

2. LECTURE 1. EXPERIMENTAL BACKGROUND AND FOUNDATIONS OF QM

Homework. Which of the operators in examples 1-7 below are bounded?

(1) The identity map

$$\mathbf{1} : \psi \mapsto \psi$$

(2) Multiplication by a coordinate

$$x_j : \psi \mapsto x_j \psi$$

$$(i.e. (x_j \psi)(x) = x_j \psi(x))$$

(3) Multiplication by a continuous function $V : \mathbb{R}^d \rightarrow \mathbb{C}$

$$V : \psi \mapsto V \psi$$

$$(again meaning (V\psi)(x) = V(x)\psi(x)).$$

(4) The momentum operator (differentiation)

$$p_j : \psi \mapsto -i\hbar \partial_j \psi$$

(5) The Laplacian

$$\Delta : \psi \mapsto \sum_{j=1}^d \partial_j^2 \psi$$

(6) A Schrödinger operator

$$H : \psi \mapsto -\frac{\hbar^2}{2m} \Delta \psi + V \psi$$

(7) An integral operator

$$K : \psi \mapsto \int K(\cdot, y) \psi(y) dy$$

$$(i.e. (K\psi)(x) = \int K(x, y) \psi(y) dy). \text{ The function } K : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{C} \text{ is called the integral kernel of the operator } K.$$

In each case, we can simply choose $D(A)$ to be the obvious domain $D(A) := \{\psi \in L^2(\mathbb{R}^d) \mid A\psi \in L^2(\mathbb{R}^d)\}$. In the last example assume that $\int |K(x, y)|^2 dx dy < \infty$. For those which are not bounded find domains of definition.

Homework. Show that the properties

$$Au = 0 \implies u = 0. \tag{1}$$

and

$$\text{Ran}(A) = \mathcal{H}. \tag{2}$$

imply that A is invertible.

Homework. Show that if operators A and C are invertible, then so is AC , with $(AC)^{-1} = C^{-1}A^{-1}$.

Homework. Assume the operator A is invertible, and the operator B is bounded and satisfies $\|B\| < \|A^{-1}\|^{-1}$.

(1) Show that the series

$$\sum_{n=0}^{\infty} (-A^{-1}B)^n,$$

called a Neumann series, is absolutely convergent (i.e. $\sum_{n=0}^{\infty} \|(-A^{-1}B)^n\| < \infty$) and provides the inverse of the operator $\mathbf{1} + A^{-1}B$.

(2) Show that the operator $A + B$, defined on $D(A + B) = D(A)$ is invertible.

3. SUPPLEMENTARY NOTES TO LECTURE 1

3.1. Experiments. I will not describe historical development of Quantum Mechanics, but rather mention two dramatic experiments. The first one was conducted by E.Rutherford in 1911 and it established the planetary model of an atom with a tiny nucleus ($10^{-13} - 10^{-12}$ cm) at the center and with electrons orbiting around it. The electrons are attracted to the nucleus and repelled by each other via the Coulomb forces. The size of an atom, i.e. the size of electron orbits is about 10^{-8} cm. The problem is that in Quantum Physics this model is unstable.

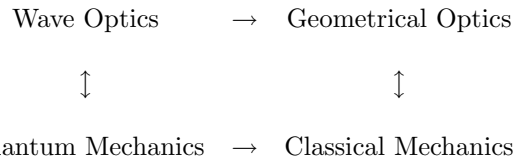
The second experiment is that on scattering electrons on a crystal conducted by Davisson and Germer (1927), G.P. Thomson (1928) and Rupp (1928). This experiment is similar to the 1805 Young's experiment confirming the wave nature of light. It can be abstracted as the double-slit experiment described below.

Theoretical ideas:

quantization of emission and absorption of the black-body radiation (to avoid the UV catastrophe, M. Planck, 1900)

notion of a quantum particle - photon (A. Einstein, 1905).

3.2. Wave Optics → Geometric Optics. We use the correspondence principle to find the form of the operator A . Here we are guided by the analogy with the wave optics transition to geometrical optics.



In every day experience we see light propagating along straight lines in accordance with the laws of geometrical optics, i.e., along the characteristics of the equation

$$\frac{\partial \phi}{\partial t} = \pm c |\nabla_x \phi| \quad (c = \text{speed of light}), \tag{3}$$

known as the *eikonal equation*. On the other hand we know that light, like electro-magnetic radiation in general, obeys Maxwell's equation which can be reduced to the wave equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \Delta u \tag{4}$$

(say for the electric field in complex representation).

The eikonal equation appears as a high frequency limit of the wave equation when the wave length is much smaller than the typical size of objects. Namely we set $u = ae^{\frac{i\phi}{\lambda}}$, where a and ϕ are real and $O(1)$ and $\lambda > 0$ is the typical wave length. ϕ is called the eikonal. Substitute this into (4) to obtain

$$\ddot{a} + 2i\lambda^{-1}\dot{a}\dot{\phi} - \lambda^{-2}a\dot{\phi}^2 + i\lambda^{-1}a\ddot{\phi} = c^2(\Delta a + 2i\lambda^{-1}\nabla a \cdot \nabla \phi - \lambda^{-2}a|\nabla \phi|^2 + \lambda^{-1}a\Delta \phi).$$

In the short wave approximation, $\lambda \ll 1$ ($\partial^\alpha a = O(1)$ and $\partial^\alpha \phi = O(1)$), we obtain

$$-a\dot{\phi}^2 = -c^2a|\nabla \phi|^2 \quad (\text{eikonal equation})$$

and

$$2\dot{a}\phi + a\ddot{\phi} = c^2(2\nabla a \cdot \nabla \phi + a\Delta \phi) \quad (\text{transport equation}).$$

An equation in Quantum Mechanics analogous to the eikonal equation is the Hamilton-Jacobi equation

$$\frac{\partial S}{\partial t} = -h(x, \nabla S), \tag{5}$$

where $h(x, k) = \frac{1}{2m}|k|^2 + V(x)$ is the classical Hamiltonian function. We would like to find an evolution equation which would lead to the Hamilton-Jacobi equation in the way the wave equation led to the eikonal one. We look for solution to the Schrödinger equation in the form $\psi(x, t) = a(x, t)e^{S(x, t)/\hbar}$, where $S(x, t)$ satisfies the Hamilton-Jacobi equation (5) and \hbar is a small parameter of the dimension of action.

Assuming a , S , and their derivatives are of order one in \hbar , then it is easy to show that, to the leading order in \hbar , ψ satisfies the equation

$$i\hbar \frac{\partial}{\partial t} \psi(x, t) = -\frac{\hbar^2}{2m} \Delta_x \psi(x, t) + V(x)\psi(x, t). \tag{6}$$

This equation is of the desired form discussed in the main text. In fact it is the correct equation, and is called the *Schrödinger equation*. The operator $\Delta = \sum_{j=1}^3 \partial_j^2$ is the *Laplacian* (in spatial dimension 3). The small constant \hbar is *Planck's constant*; it is one of the fundamental constants in nature.

4. LECTURES 2-3. EXISTENCE OF DYNAMICS AND SELF-ADJOINTNESS

Homework. Let A be a bounded operator. Using the power series representation, show that

$$(1) \quad e^{isA}|_{s=0} = \mathbf{1}; \tag{7}$$

$$(2) \quad e^{isA}e^{itA} = e^{i(s+t)A}; \tag{8}$$

$$(3) \quad \frac{\partial}{\partial s}e^{isA} = iAe^{isA} = e^{isA}iA; \tag{9}$$

$$(4) \text{ if } A \text{ is self-adjoint, then } e^{iA} \text{ is an } \textit{isometry}; \tag{10}$$

$$\|e^{iA}\psi\| = \|\psi\|.$$

Homework. Show that if A is self-adjoint bounded, then e^{iA} is unitary.

Homework. Show that if $\phi : \mathbb{R}^d \rightarrow \mathbb{R}$ is continuous, then the operator

$$U : \psi \mapsto e^{i\phi}\psi$$

is unitary on $L^2(\mathbb{R}^d)$.

Homework. Show that under \mathcal{F}

- (1) $e^{-\frac{|x|^2}{2a\hbar^2}} \mapsto (\hbar a)^{d/2} e^{-\frac{a|k|^2}{2}} \quad (Re(a) > 0)$. Hint: try $d = 1$ first – complete the square in the exponent and move the contour of integration in the complex plane.
- (2) $e^{-\frac{1}{2\hbar^2}x \cdot A^{-1}x} \mapsto \hbar^{d/2}(\det A)^{1/2} e^{-\frac{1}{2}k \cdot Ak}$ (A a positive $d \times d$ matrix). Hint: diagonalize and use the previous result.
- (3) $\sqrt{\frac{\pi}{2\hbar}} \frac{e^{-\sqrt{b/\hbar^2}|x|}}{|x|} \mapsto (|k|^2 + b)^{-1} \quad (b > 0, d = 3)$. Hint: use spherical coordinates. Alternatively, see Problem ?? below.
- (4) Show that for $b > 0$ and $d = 3$, under \mathcal{F}^{-1} ,

$$(|k|^2 + b)^{-1} \mapsto \sqrt{\frac{\pi}{2\hbar}} \frac{e^{-\sqrt{b/\hbar^2}|x|}}{|x|}$$

(hint: use spherical coordinates, then contour deformation and residue theory).

In the first example, if $Re(a) > 0$ then the function on the left is in $L^1(\mathbb{R}^d)$, and the Fourier transform is well-defined. However, we can extend this result to $Re(a) = 0$, in which case the integral is convergent, but not absolutely convergent.

For the next four statements, suppose $\psi, \phi \in C_0^\infty(\mathbb{R}^d)$.

- (1) $-i\hbar \widehat{\nabla_x \psi}(k) = k \hat{\psi}(k)$.
- (2) $x \hat{\psi}(k) = i\hbar \nabla_k \hat{\psi}(k)$.
- (3) $\widehat{\phi \psi} = (2\pi\hbar)^{-d/2} \hat{\phi} * \hat{\psi}$.
- (4) $\widehat{\phi * \psi} = (2\pi\hbar)^{d/2} \hat{\phi} \hat{\psi}$.

Here

$$(f * g)(x) := \int_{\mathbb{R}^d} f(y)g(x - y)dy$$

is the *convolution* of f and g . The last four properties can be loosely summarized by saying that the Fourier transform exchanges differentiation and coordinate multiplication, and products and convolutions.

Homework. (1) Show that under \mathcal{F}^{-1} ,

$$\delta(k - a) \mapsto (2\pi\hbar)^{-d/2} e^{ia \cdot x / \hbar}.$$

Here δ is the *Dirac delta function* – not really a function, but a *distribution* – characterized by the property $\int f(x)\delta(x - a)dx = f(a)$. The exponential function on the right hand side is called a *plane wave*.

Homework. Let $H_0 := (-\frac{\hbar^2}{2m}\Delta, \lambda > 0$, and $d = 3$. Show that

$$((H_0 + \lambda)^{-1}\psi)(x) = \frac{m}{2\pi\hbar^2} \int_{\mathbb{R}^3} \frac{e^{-\frac{\sqrt{2m\lambda}}{\hbar}|x-y|}}{|x-y|} \psi(y) dy. \quad (11)$$

4.1. Supplementary Notes for Lecture 2. Self-adjoint Operators.

Definition 1. A linear operator A acting on a Hilbert space \mathcal{H} is *self-adjoint* if and only if A is symmetric and $\text{Ran}(A \pm i) = \mathcal{H}$.

Remark. Instead of $\text{Ran}(A \pm i) = \mathcal{H}$, we could have used in the definition

$$\text{Ran}(A \pm i\lambda) = \mathcal{H} \text{ for some } \lambda > 0.$$

Indeed, this would amount to replacing the operator A by $\lambda^{-1}A$.

Note that the condition $\text{Ran}(A \pm i) = \mathcal{H}$ is equivalent to the fact that the equation

$$(A \pm i)\psi = f \quad (12)$$

has a solution. If, in addition, A is symmetric, then this equation has a unique solution, i.e the operator $A \pm i$ is also one-to-one. The latter is equivalent to showing that $(A \pm i)\psi = 0 \rightarrow \psi = 0$. Now, assume that $(A \pm i)\psi = 0$. Then $0 = \langle (A \pm i)\psi, \phi \rangle = \langle \psi, (A \mp i)\phi \rangle \forall \phi \in \mathcal{H}$. Since $(A \mp i)\phi$ runs over all \mathcal{H} as ϕ runs over \mathcal{H} , we conclude that $\psi = 0$. This shows that the operator $A \pm i$ is one-to-one and (12) has a unique solution.

Examples. $x_j, -i\hbar\partial_{x_j}, f(x)$ and $f(p)$ for f real and bounded, integral operators $Kf(x) = \int K(x, y)f(y) dy$ with $K(x, y) = \overline{K(y, x)}$ and, say, $K \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$, are all self-adjoint.

Proof. We show this for $-i\hbar\partial_x$. This operator is symmetric, so we compute $\text{Ran}(-i\hbar\partial_x + i)$. Solve

$$(-i\hbar\partial_x + i)\psi = f,$$

which, by the \hbar -Fourier transform, is equivalent to

$$(k + i)\hat{\psi} = \hat{f},$$

and therefore

$$\psi = (2\pi\hbar)^{-3/2} \int e^{ikx/\hbar} \frac{\hat{f}(k)}{k + i} dk.$$

Now for all $f \in L^2, \psi \in H_1 = \mathcal{D}(-i\hbar\partial_x)$ and therefore $\text{Ran}(-i\hbar\partial_x + i) = L^2$. Similarly $\text{Ran}(-i\hbar\partial_x - i) = L^2$. \square

Homework. Show that $x_j, f(x)$ and $f(p)$, for f real and bounded, Δ are self-adjoint.

Below we will often use the following fact

Homework. Show that if $\|K\| < 1$, then the operator $1 + K$ is invertible and its inverse is given by the absolutely convergent $(\sum_{n=0}^{\infty} \|K^n\| < \infty)$ series

$$\sum_{n=0}^{\infty} (-K)^n \quad (\text{Neumann series}).$$

Theorem 2. *If A is symmetric and bounded, then A is self-adjoint.*

Proof. We show that $\text{Ran}(A + i\lambda) = \mathcal{H}$, provided $|\lambda|$ is sufficiently large. This is equivalent to solving the equation

$$(A + i\lambda)\psi = f \quad (13)$$

for all $f \in \mathcal{H}$ and such a λ . Now, divide this equation by $i\lambda$ to obtain

$$\psi + K(\lambda)\psi = g,$$

where $K(\lambda) = (i\lambda)^{-1}A$ and $g = (i\lambda)^{-1}f$. Let $|\lambda| > \|V\|$. Then $\|K(\lambda)\| = \frac{1}{|\lambda|} \|A\| < 1$ and we conclude that $1 + K(\lambda)$ is invertible, as shown in the homework above. Therefore

$$\psi = (1 + K(\lambda))^{-1}g = \sum (-K(\lambda))^n g \in L^2.$$

\square

Homework. Show that integral operators $Kf(x) = \int K(x, y)f(y) dy$ with $K(x, y) = \overline{K(y, x)}$ and $K \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$ are self-adjoint.

Theorem 3. *If A is self-adjoint, then $A - z$ is invertible for all z with $\text{Im } z \neq 0$, and*

$$\|(A - z)^{-1}\| \leq \frac{1}{|\text{Im } z|} \quad (14)$$

Proof. $\text{Null}(A - z) = \{0\}$ and $\text{Ran}(A - z) = \mathcal{H}$ imply that $A - z$ is invertible. Now write $z = \lambda + i\mu$ with $\lambda, \mu \in \mathbb{R}$. Then

$$\|(A - z)u\|^2 = \|(A - \lambda)u\|^2 + \|\mu u\|^2 \geq |\mu| \|u\|^2,$$

which implies (14) if one defines $v := (A - z)u$. \square

Theorem 4. *Assume that V is real and bounded. Then $H := -\frac{\hbar^2}{2m}\Delta + V(x)$, with $\mathcal{D}(H) = \mathcal{D}(\Delta)$, is self-adjoint.*

Proof. Since H is symmetric, it suffices to show that $\text{Ran}(H \pm i) = \mathcal{H}$. We want to solve the equation

$$(H + i\lambda)\psi = f \quad (15)$$

for all $f \in \mathcal{H}$ and some $\lambda \neq 0$. Write $H_0 = -\frac{\hbar^2}{2m}\Delta$. We know that $H_0 \pm i\lambda$ is one-to-one and onto, and therefore invertible. Multiplying (15) by $(H_0 + i\lambda)^{-1}$, we find

$$\psi + K(\lambda)\psi = g,$$

where $K(\lambda) = (H_0 + i\lambda)^{-1}V$ and $g = (H_0 + i\lambda)^{-1}f$. By Theorem 3,

$$\|K(\lambda)\| \leq \frac{1}{|\lambda|} \|V\|.$$

Thus, for $|\lambda| > \|V\|$, $\|K(\lambda)\| < 1$ and therefore $1 + K(\lambda)$ is invertible, as shown in the homework above. Therefore

$$\psi = (1 + K(\lambda))^{-1}g = \sum (-K(\lambda))^n g \in L^2.$$

Moreover,

$$(H_0 + i\lambda)\psi = \sum (-K(\lambda)^T)^n f \in L^2,$$

where $K(\lambda)^T = V(H + i\lambda)^{-1}$ (**Homework:** show this). So $\psi \in \mathcal{D}(H_0) = \mathcal{D}(H)$. Hence $\text{Ran}(H + i\lambda) = \mathcal{H}$ and H is self-adjoint. \square

Remark. Coulomb potential $\frac{\alpha}{|x|}$ is not bounded. We can extend the theorem to a more general class of potentials V satisfying for all $\psi \in \mathcal{D}(H_0)$

$$\|V\psi\| \leq a\|H_0\psi\| + b\|\psi\| \quad (16)$$

with $a < 1$ (H_0 -bounded potentials).

Homework. Show that $V(x) = \frac{\alpha}{|x|}$ satisfies (16). *Hint:* Write $V(x) = V_1(x) + V_2(x)$ where

$$V_1(x) = \begin{cases} V(x) & |x| \leq 1 \\ 0 & |x| > 1 \end{cases}, \quad V_2(x) = \begin{cases} 0 & |x| \leq 1 \\ V(x) & |x| > 1. \end{cases}$$

Homework. Prove that the operator $H := -\frac{\hbar^2}{2m}\Delta - \frac{\alpha}{|x|}$ (the Schrödinger operator of the hydrogen atom with the infinitely heavy nucleus) is self-adjoint.

5. LECTURE 4. QUANTUM OBSERVABLES, QUANTIZATION AND CONSERVATION LAWS

Homework. *Check that for any observable, A , we have*

$$\frac{d}{dt}\langle A \rangle_\psi = \langle \psi, \frac{i}{\hbar}[H, A]\psi \rangle.$$

Homework. Let

$$A(t) := e^{itH/\hbar} A e^{-itH/\hbar}.$$

(1) Let ψ be the solution of Schrödinger's equation with initial condition ψ_0 : $\psi(t) = e^{-itH/\hbar}\psi_0$. Prove that

$$\langle A \rangle_{\psi(t)} = \langle A(t) \rangle_{\psi_0}. \quad (17)$$

(2) Prove that

$$\frac{d}{dt}A(t) = \frac{i}{\hbar}[H, A(t)].$$

$$(3) \quad m\dot{x}(t) = p(t). \tag{18}$$

$$(4) \quad \dot{p}(t) = -\nabla V(x(t)). \tag{19}$$

6. CONSERVATION LAWS

If an observable A commutes with the Schrödinger operator H , i. e. $[A, H] = 0$, then its average in any evolving state $\psi(t)$ is independent of t :

$$\langle A \rangle_{\psi(t)} = \langle A(t) \rangle_{\psi} = \langle A \rangle_{\psi}, \tag{20}$$

where $\psi = \psi(0)$. For example, since obviously $[H, H] = 0$, we also have $\langle H \rangle_{\psi(t)} = \text{constant}$, which is the mean-value version of the conservation of energy.

Most of conservation laws come from symmetries of the quantum system in question. For example

- Time translation invariance (V is independent of t) \rightarrow conservation of energy
- Space translation invariance (V is independent of x) \rightarrow conservation of momentum
- Space rotation invariance (V is rotation invariant, i.e. is a function of $|x|$) \rightarrow conservation of angular momentum
- Gauge invariance (invariance of the equation under the transformation $\psi \rightarrow e^{i\alpha}\psi$) \rightarrow conservation of charge/probability.

Symmetries can be associated with one-parameter groups U_s of unitary operators. We say that U_s is a symmetry iff

$$\psi_t \text{ is a solution to SE } \rightarrow U_s \psi_t \text{ is a solution to SE.}$$

Let A be a generator of a one-parameter group U_s : $\partial_t U_s = iAU_s$. Then

$$U_s \text{ is a symmetry of SE } \rightarrow A \text{ commutes with } H.$$

Indeed, the fact that U_s is a symmetry implies that $i\hbar\partial_t U_s \psi_t = H U_s \psi_t$. Inverting U_s gives $i\hbar\partial_t \psi_t = U_s^{-1} H U_s \psi_t$. Differentiating the last equation w.r.to s and setting $s = 0$ and $t = 0$ we arrive at $i[H, A]\psi = 0$, where $\psi = \psi(0)$. Since this is true for all ψ we conclude that $[H, A] = 0$, i. e. A commutes with H .

Examples of symmetry groups and their generators:

- Spacial translations: $U_y : \psi(x) \rightarrow \psi(x + y)$, $y \in \mathbb{R}^3$ with the generator $\frac{p}{\hbar} = -i\nabla_x \rightarrow$ conservation of momentum
- Spacial rotation: $U_R : \psi(x) \rightarrow \psi(Rx)$, $R \in O(3)$ with the generator $\frac{L}{\hbar} = \frac{x \times p}{\hbar} \rightarrow$ conservation of angular momentum
- Gauge invariance: $U_\alpha : \psi(x) \rightarrow e^{i\alpha}\psi(x)$, $\alpha \in \mathbb{R}$ with the generator $i \rightarrow$ conservation of charge/probability.

Differential form of conservation laws and currents.

7. LECTURE 5. UNCERTAINTY PRINCIPLE

8. LECTURE 6. THE SPECTRUM OF SCHRÖDINGER OPERATORS

Homework. Prove that as operators on $L^2(\mathbb{R}^d)$,

- (1) $\sigma(\mathbf{1}) = \{1\}$.
- (2) $\sigma(p_j) = \mathbb{R}$.
- (3) $\sigma(x_j) = \mathbb{R}$.
- (4) $\sigma(V) = \overline{\text{range}(V)}$, where V is the multiplication operator on $L^2(\mathbb{R}^d)$ by a continuous function $V(x) : \mathbb{R}^d \rightarrow \mathbb{C}$.
- (5) $\sigma(-\Delta) = [0, \infty)$.
- (6) $\sigma(f(p)) = \overline{\text{range}(f)}$, where $f(p) := \mathcal{F}^{-1} f \mathcal{F}$ with $f(k)$, the multiplication operator on $L^2(\mathbb{R}^d)$ by a continuous function $f(k) : \mathbb{R}^d \rightarrow \mathbb{C}$.

Homework. (1) Show $\text{Null}(A - \lambda)$ is a vector space.

(2) Show that if $A = A^*$, eigenvectors of A corresponding to different eigenvalues are orthogonal.

Homework. Considering the operators x_j and p_j on $L^2(\mathbb{R}^d)$ show that

- (1) $\sigma_{ess}(p_j) = \sigma(p_j) = \mathbb{R}$;
- (2) $\sigma_{ess}(x_j) = \sigma(x_j) = \mathbb{R}$;
- (3) $\sigma_{ess}(-\Delta) = \sigma(-\Delta) = [0, \infty)$.

Hint: Show that these operators do not have discrete spectrum.

Homework. Show that if $U : \mathcal{H} \rightarrow \mathcal{H}$ is unitary, then $\sigma(U^*AU) = \sigma(A)$, $\sigma_d(U^*AU) = \sigma_d(A)$, and $\sigma_{ess}(U^*AU) = \sigma_{ess}(A)$.

Homework. Let A be a self-adjoint operator on \mathcal{H} . If λ is an accumulation point of $\sigma(A)$, then $\lambda \in \sigma_{ess}(A)$. Hint: use the definition of the essential spectrum.

Homework. Let $V(x) := \alpha/|x|$, with $\alpha \in \mathbb{R}$. Show that

- (1) $\sigma_{ess}(H) = [0, \infty)$;
- (2) H can have only negative isolated eigenvalues, possibly accumulating at 0;
- (3) H has at least one negative eigenvalue.

Homework. Let $V(x) = 5|x|^4$. Show that the discrete spectrum of $H = -\Delta + V$ on $L^2(\mathbb{R}^3)$ is not empty.

Homework. Assume A is a self-adjoint operator. Show that

- (1) If W is invariant under A , then so is W^\perp ;
- (2) The span of the eigenfunctions of A and its orthogonal complement are invariant under A ;
- (3) The restriction operator

$$A|_{\{\text{span of eigenfunctions of } A\}}$$

has a purely discrete spectrum;

- (4) The restriction operator

$$A|_{\{\text{span of eigenfunctions of } A\}^\perp}$$

has a purely essential spectrum.

Homework. Show the Schrödinger operator describing the Hydrogen atom

$$H = -\frac{\hbar^2}{2m}\Delta - \frac{e^2}{|x|},$$

acting on the Hilbert space $L^2(\mathbb{R}^3)$, has an isolated eigenvalue of finite multiplicity at the bottom, $\inf \sigma(H)$, of its spectrum.

9. ADDITIONAL MATERIAL ON SPECTRAL THEORY: SPREADING SEQUENCES

Definition 5. Let H be a selfadjoint operator, and λ be a real number. A sequence ψ_n of elements in $L^2(\mathbb{R}^3)$ is called a spreading sequence for H and λ if

- 1) $\|\psi_n\| = 1$
- 2) $\|(H - \lambda)\psi_n\| \rightarrow 0$
- 3) For every $\Omega \subset \mathbb{R}^3$ bounded, $\text{supp}(\psi_n) \cap \Omega = \emptyset$ if n is large enough.

Theorem 6. Let $H = -\Delta + V$ be a self-adjoint operator where V is bounded from below. Then $\lambda \in \sigma_{ess}(H)$ if and only if there exists a spreading sequence for H and λ .

Proof. Let $\{\psi_n\}$ be a spreading sequence for H and λ and let $\phi_n = \frac{(H-\lambda)\psi_n}{\|(H-\lambda)\psi_n\|}$. Evidently, $\|\phi_n\| = 1$. Since $(H - \lambda)^{-1}\phi_n = \frac{\psi_n}{\|(H-\lambda)\psi_n\|}$, and $\|(H - \lambda)\psi_n\| \rightarrow 0$, we obtain that $\|(H - \lambda)^{-1}\phi_n\| \rightarrow \infty$. Therefore $H - \lambda$ is unbounded which implies that $\lambda \in \sigma(H)$. We will prove that $\lambda \notin \sigma_d(H)$. To prove that suppose that $\lambda \in \sigma_d(H)$. Let M denote the eigenspace of λ . Then $(H - \lambda)$ is invertible on M^\perp . Let P and P^\perp be the orthogonal projections on M and M^\perp , respectively. We have $P + P^\perp = \mathbf{1}$. Then $\|P\psi_n\| \rightarrow 0$ and using $\frac{P^\perp\psi_n}{\|P^\perp\psi_n\|}$ we can show that $(H - \lambda)$ is not invertible on M^\perp , a contradiction. Hence $\lambda \notin \sigma_d(H)$ and therefore $\lambda \in \sigma_{ess}(H)$.

Suppose now that $\lambda \in \sigma_{ess}(H)$. Then there is a sequence ϕ_n with $\|\phi_n\| = 1$ and $\|(H - \lambda)^{-1}\phi_n\| \rightarrow \infty$. Let $\psi_n = \frac{(H-\lambda)^{-1}\phi_n}{\|(H-\lambda)^{-1}\phi_n\|}$. We claim that for every bounded set Ω we have that $\|\chi_\Omega\psi_n\| \rightarrow 0$ as $n \rightarrow \infty$. Indeed, we can assume without loss of generality that $V \geq 0$ which implies that $(H + 1)$ is invertible.

$$\chi_\Omega\psi_n = \chi_\Omega(-\Delta + 1)^{-1}(-\Delta + 1)(H + 1)^{-1}(H + 1)\psi_n. \quad (21)$$

On the other hand we have that

$$B := (-\Delta + 1)(H + 1)^{-1} = 1 - V(H + 1)^{-1}, \quad (22)$$

so B is bounded. Now, we have

$$\chi_\Omega(-\Delta + 1)^{-1}f = \int K(x, y)f(y)dy, \quad (23)$$

with $K \in L^2(\mathbb{R}^3 \otimes \mathbb{R}^3)$.

Homework. Show that $K(x, y) = \chi_\Omega(x)G(x - y)$, where $G(y) = C \frac{e^{-|y|}}{|y|}$ and C is a constant.

Let $K_x(y) := K(x, y)$. Using that

$$(H + 1)\psi_n = \frac{\phi_n}{\|(H - \lambda)^{-1}\phi_n\|} + (\lambda + 1)\psi_n \quad (24)$$

we obtain that

$$\begin{aligned} \chi_\Omega \psi_n &= \chi_\Omega(-\Delta + 1)^{-1}B(\lambda + 1)\psi_n + \chi_\Omega(-\Delta + 1)^{-1}B \frac{\phi_n}{\|(H - \lambda)^{-1}\phi_n\|} \\ &= \langle K_x, B(\lambda + 1)\psi_n \rangle + \chi_\Omega(-\Delta + 1)^{-1}B \frac{\phi_n}{\|(H - \lambda)^{-1}\phi_n\|}. \end{aligned} \quad (25)$$

We have that

$$\|\chi_\Omega(-\Delta + 1)^{-1}B \frac{\phi_n}{\|(H - \lambda)^{-1}\phi_n\|}\| \leq \|B\| \left\| \frac{\phi_n}{\|(H - \lambda)^{-1}\phi_n\|} \right\| \rightarrow 0. \quad (26)$$

On the other hand, since $\{\psi_n\}$ is a spreading sequence, we have that $\forall x, \langle B^*K_x, \psi_n \rangle \rightarrow 0$ and therefore

$$\|\langle K_x, B(\lambda + 1)\psi_n \rangle\|_x = |\lambda + 1| \|\langle B^*K_x, \psi_n \rangle\|_x \rightarrow 0.$$

Hence we conclude that for any bounded set $\Omega \subset \mathbb{R}^3$ we have

$$\|\chi_\Omega \phi_n\| \rightarrow 0. \quad (27)$$

Let $B(R)$ be a ball of radius R centered at the origin and let $R_m \rightarrow \infty$ as $m \rightarrow \infty$. Since $\|\chi_\Omega \psi_n\| \rightarrow 0$ as $n \rightarrow \infty$ for any bounded set Ω we have that $\forall m, \|\chi_{B(R_m)} \psi_n\| \rightarrow 0$ as $n \rightarrow \infty$. Hence using a diagonal procedure and passing to a subsequence, if necessary, we obtain that $\|\chi_{B(R_m(n))} \psi_n\| \rightarrow 0$ as $n \rightarrow \infty$ for some subsequence $m(n) \rightarrow \infty$ with $n \rightarrow \infty$. Let $f_n = \frac{(1 - \chi_{B(R_m(n))})\psi_n}{\|(1 - \chi_{B(R_m(n))})\psi_n\|}$. Evidently $\|f_n\| = 1$ and $\text{supp}(f_n) \cap \Omega = \emptyset$ for all bounded Ω provided that n is large. To finish the proof it suffices to show that

$$\|(H - \lambda)f_n\| \rightarrow 0. \quad (28)$$

Homework. Show the last relation.

Hence f_n is a spreading sequence for H and λ . □

10. LECTURE 7. QUANTUM STATISTICS

Homework. Let the vectors ψ_n evolve according to the Schrödinger equation, $i\hbar \frac{\partial \psi}{\partial t} = H\psi$. Show that the density matrix $\rho = \sum p_n P_{\psi_n}$ satisfies the equation

$$i \frac{\partial \rho}{\partial t} = \frac{1}{\hbar} [H, \rho]. \quad (29)$$

Homework. Let H be a bounded operator and f , real analytic function. Show that operator $f(H)$ is a static solution of equation (29).

Homework. Let ψ_i be normalized eigenfunctions of H (i.e. $H\psi_i = \lambda_i \psi_i$). Show that $\rho = \sum_i p_i P_{\psi_i}$, for any $p_i \geq 0, \sum p_i < \infty$, independent of t , is a static solutions of the equation $i \frac{\partial \rho}{\partial t} = \frac{1}{\hbar} [H, \rho]$.

Homework. Let ρ be the integral operator with the integral kernel

$$\rho(x, x') = \int \overline{\psi(x, y)} \psi(x', y) dy. \quad (30)$$

Show that for any operator A acting on the variable x ,

$$\langle \psi, A\psi \rangle = \text{tr}(A\rho). \quad (31)$$

Homework. Let P_ψ be the rank-one projection on the normalized wave function ψ . Show that $\text{tr}(AP_\psi) = \langle \psi, A\psi \rangle$.

Homework. Let P be orthogonal projection. Show that

- 1) $\|P\| = 1$
- 2) $1 - P$ orthogonal projection
- 3) $\text{Ran}P = \text{Ran}(I - P)$.

Homework: $V \subset L^2$ closed vector subspace. Then there exists an orthogonal projection P_V such that $RanP_V = V$.

Homework: If P is an orthogonal projection then $RanP$ is a closed subspace of L^2 .

Homework: Let P_ψ be the orthogonal projection onto ψ . Show that $P_\psi \geq 0$ and $\sigma(P_\psi) = \{0, 1\}$.

Homework: Let K be an operator. If there exists an orthonormal basis (ψ_n) such that $\sum_{n=1}^{\infty} \langle \psi_n, \sqrt{K^*K} \psi_n \rangle < \infty$, then the quantity

$$Tr(K) := \sum_{n=1}^{\infty} \langle \psi_n, K \psi_n \rangle \quad (32)$$

is independent of the choice of basis.

Homework: Show the following properties of trace:

1) $Tr(\alpha A + \beta B) = \alpha Tr A + \beta Tr B$.

2) If A is a bounded and B is a trace class operator, then $Tr(AB) = Tr(BA)$.

3) $Tr A^* = \overline{Tr A}$

4) If $K\psi(x) = \int K(x, y)\psi(y)dy$, then $Tr K = \int K(x, x)dx$.

Homework: Let $\|\psi\| = 1$ and P_ψ orthogonal projection onto ψ . Then $Tr(AP_\psi) = \langle \psi, A\psi \rangle$.

Homework: Let $\rho = \sum_{n=1}^{\infty} p_n P_{\psi_n}$, where $p_n \geq 0$ and $\sum p_n = 1$. Show that $\rho \geq 0$, $Tr\rho = 1$ and $\sigma(\rho) = \{0, p_1, p_2, \dots\}$.

Homework: Check that if $\rho = P_\psi$, then $\rho(x, x) = |\psi(x)|^2$, and $\hat{\rho}(k, k) = |\hat{\psi}(k)|^2$, where $\hat{\rho}(k_1, k_2)$ is the Fourier transform of $\rho(x, y)$.

Properties of trace norm

$$\|A\|_1 = \sup \frac{|Tr(AB)|}{\|B\|}, \quad (33)$$

$$\|AB\|_1 \leq \|A\|_1 \|B\|, \quad (34)$$

$$\|A\| \leq Tr|A| \quad (35)$$

$$\|A \otimes B\|_1 \leq \|A\|_1 \|B\|_1 \quad (36)$$

Distance: $\|A - B\|_1, d_F(A, B) = \min\{\|\Psi - \Phi\| | Tr_{env} P_\Psi = A, Tr_{env} P_\Phi = B\}$.

11. LECTURE 8. OPEN SYSTEMS

Assume our system interacts with environment. The total system

$$TS = T + E,$$

is described by a density operator R . Assume that we do not know anything about the state of environment and do observations only on the system. What is the state of the system which gives the results of these observations? it is the reduced density matrix $\rho = Tr_{env} R$, which is given in terms of the partial trace Tr_{env} of R over the environment variables. This partial trace is defined either by

$$R \leftrightarrow R(x, y, x', y') \implies \rho \leftrightarrow \rho(x, x') \text{ with } \rho(x, x') := \int R(x, y, x', y) dy, \quad (37)$$

or by

$$\langle \phi, Tr_{env} R \psi \rangle = \sum_i \langle \phi \chi_i, R \psi \chi_i \rangle, \quad (38)$$

for any $\phi, \psi \in L^2(dx)$ and for any orthonormal basis $\{\chi_j\}$ in $L^2(dy)$.

Homework: Check that the definitions of partial trace given by (37) and (38) are equivalent.

Homework: Show that for any system observable A we have

$$Tr(AR) = Tr_{syst}(A\rho), \quad \rho = Tr_{env} R. \quad (39)$$

Remark. In tensor product notation we write $\phi \otimes \chi_i$, and $A \otimes I$ for a system observable A acting only on x .

Reconstruction of a pure state:

Theorem 7. Given density matrix ρ there exists a Hilbert space \mathcal{H}_e and the vector $\psi \in \mathcal{H} \otimes \mathcal{H}_e$ such that

$$\rho = Tr_e P_\psi. \quad (40)$$

Proof. Let ϕ_j and p_j be the complete system of orthonormal eigenfunctions of $\sqrt{\rho}$ and the corresponding them eigenvalues so that we have the spectral decomposition $\sqrt{\rho} = \sum_j p_j |\phi_j\rangle\langle\phi_j|$. We choose

$$\psi = \sum \sqrt{p_j} \phi_j \otimes \bar{\phi}_j \in \mathcal{H} \otimes \mathcal{H}^*.$$

Then, if $\mathcal{H}_e = \mathcal{H}^*$, we have $Tr_e P_\psi = \rho$. □

12. REDUCED DYNAMICS

Assume our total system evolved according to

$$i \frac{\partial R_t}{\partial t} = \frac{1}{\hbar} [H_{tot}, R_t], R_{t=0} = R_0, \quad (41)$$

where H_{tot} is the Schrödinger operator of the total system

$$H_{tot} = H_{syst} + H_{envir} + \lambda v \quad (42)$$

acting on $L^2(dx dy)$. Here H_{syst} and H_{envir} are Schrödinger Operators of this system and environment acting on $L^2(dx)$ and $L^2(dy)$ respectively. We know $R_t = \alpha_t(R_0)$, where $\alpha_t(R) = e^{-\frac{iH_{tot}t}{\hbar}} R e^{\frac{iH_{tot}t}{\hbar}}$.

Reduced density matrix of the system at time t is

$$\rho_t := Tr_{envir} R_t \text{ reduced evolution} \quad (43)$$

Assume that initially $R_0 = \rho_0 \otimes \rho_{envir0} \implies R_t = \alpha_t(\rho_0 \otimes \rho_{envir0})$. Define $\beta_t(\rho_0) = \rho_t$. What can we say about the reduced evolution ρ_t ?

Theorem 8. 1) β_t linear

2) β_t positive

3) β_t preserves the trace.

4) $\|\beta_t(\rho)\|_1 \leq \|\rho\|_1$

5) $\beta_t(\rho) = \sum_n V_{nt} \rho V_{nt}^*$, where V_{nt} are bounded operators and $\sum_n V_{nt}^* V_{nt} = I$ (strong convexity).

Remark. In fact 5) \implies 1)- 3).

Homework: Show this and show 1)-3) directly.

Proof. We show only the property 5). We drop the subindex t . Let $\{\chi_i\}$ be orthonormal basis in the environment space $L^2(dy)$. Then $\forall \phi, \psi \in L^2(dx)$, we have

$$\langle \phi, \beta(\rho_0) \psi \rangle = \sum_i \langle \phi \chi_i, \alpha(\rho_0 \otimes \rho_{e0}) \psi \chi_i \rangle. \quad (44)$$

Let $U := e^{-\frac{iH_{tot}t}{\hbar}}$ and χ_i be an orthonormal basis of EFs of ρ_{e0} with eigenvalues λ_j . Then $\rho_{e0} = \sum \lambda_j P_{\chi_j} = \sum \lambda_j |\chi_j\rangle\langle\chi_j|$, so that

$$\begin{aligned} & \langle \phi, \beta(\rho_0) \psi \rangle \\ &= \sum_{i,j} \langle U^* \phi \chi_i, \rho_0 \otimes \rho_{e0} U^* \psi \chi_i \rangle \\ &= \sum_{i,j} \langle \sqrt{\lambda_j} \langle \chi_j, U^* \phi \chi_i \rangle_s, \rho_0 \sqrt{\lambda_j} \langle \chi_j, U^* \psi \chi_i \rangle_s \rangle_{en} \\ &= \sum_{i,j} \langle V_{ij}^* \phi, \rho_0 V_{ij}^* \psi \rangle_{en} = \langle \phi, \sum_{i,j} V_{ij} \rho_0 V_{ij}^* \psi \rangle. \end{aligned} \quad (45)$$

where $V_{ij}^* \phi := \sqrt{\lambda_j} \langle \chi_j, U^* \phi \chi_i \rangle_s$. Now

$$\begin{aligned} & \langle V_{ij}^* \phi, \psi \rangle_s = \langle \phi, V_{ij}^* \psi \rangle_s = \sqrt{\lambda_j} \langle \phi, \langle \chi_j, U^* \psi \chi_i \rangle_{en} \rangle_s \\ &= \sqrt{\lambda_j} \langle U \phi \chi_j, \psi \chi_i \rangle = \langle \sqrt{\lambda_j} \langle U \phi \chi_j, \chi_i \rangle_{en}, \psi \rangle_s \\ &\implies V_{ij}^* \phi = \sqrt{\lambda_j} \langle \chi_i, U \phi \chi_j \rangle_{en} \\ &\implies \sum_{i,j} V_{ij}^* V_{ij} \phi = \sum_{i,j} V_{ij}^* \sqrt{\lambda_j} \langle \chi_i, U \phi \chi_j \rangle_{en} \end{aligned}$$

$$\begin{aligned}
&= \sum_{ij} \lambda_j \langle \chi_j, U^* \langle \chi_i, U \phi \chi_j \rangle_{en} \chi_i \rangle_{en}. \\
&= \sum_j \lambda_j \langle \chi_j, U^* \sum_i \langle \chi_i, U \phi \chi_j \rangle_{en} \chi_i \rangle_{en} \\
&= \sum_j \lambda_j \langle \chi_j, U^* U \phi \chi_j \rangle_{en} = \sum_j \lambda_j \langle \chi_j, \phi \chi_j \rangle_{en} \\
&= \sum_j \lambda_j \phi = \phi
\end{aligned} \tag{46}$$

Since $\sum \lambda_j = \text{Tr} \rho_{e0} = 1$. □

Definition 9. 1) Maps satisfying the conclusions of theorem 8 are called dynamical maps.
2) Evolution β_t satisfying the conclusions of theorem 8 is called dissipative evolution.
3) A dissipative evolution β_t is called Markov iff

$$\beta_t \circ \beta_s = \beta_{t+s} \quad \forall t, s \geq 0. \tag{47}$$

For a Markov dissipative evolution β_t we define the generator by

$$K(\rho) := \partial_t \beta_t |_{t=0},$$

so that

$$\partial_t \beta_t(\rho) = K(\beta_t(\rho)).$$

Theorem 10. *Generators of Markov dissipative evolutions are of the form*

$$K(\rho) = -i[H, \rho] + \sum_{j=0}^{\infty} (W_j \rho W_j^* - \frac{1}{2} \{W_j^* W_j, \rho\}) \tag{48}$$

where H is self-adjoint, $\{A, B\} : AB + BA$ and $\sum W_j^* W_j$ converges strongly.

13. DUAL REDUCED EVOLUTION

Recall coupling between density matrices and observables:

$$\langle \rho, A \rangle = \text{Tr}_{\text{sys}}(A\rho). \tag{49}$$

Define the reduced evolution of observables by

$$\langle \rho, \beta_t^*(A) \rangle = \langle \beta_t(\rho), A \rangle. \tag{50}$$

β_t Markov $\implies \beta_t^*$ Markov $\implies \frac{\partial}{\partial t} \beta_t^* = \mathcal{L} \beta_t^*$ (with $\mathcal{L} = K^* \implies$) generator of Markov dissipative evolution of observables

$$\mathcal{L}(A) = i[H, A] + \sum_i (W_j^* A W_j - \frac{1}{2} \{W_j^* W_j, A\}). \tag{51}$$

Maps satisfying the conclusions of theorem 8 are called dynamical maps.

Qn: Do processes in environment affect ρ_s ?

Answer: no, in the sense that for every unitary $W \in B(\mathcal{H}_e)$ and $V \in B(\mathcal{H}_s)$,

$$\text{Tr}_{\text{environ}}(V \otimes W R V^* \otimes W^*) = V(\text{Tr}_{\text{environ}} R) V^*, \text{ independent of } W. \tag{52}$$

Homework: Show this.

β is said to be irreversible $\leftrightarrow \beta$ is not invertible.

If $\beta(\rho) = U \rho U^*$ where U unitary then β is reversible.

Theorem 11. (Wigner) *If $\exists \Phi : \text{operators} \rightarrow \text{operators}$, one-to-one and onto, such that*

$$\text{Tr}(\beta(\rho) \phi(A)) = \text{Tr}(\rho A) \quad \forall A \in B(H), \tag{53}$$

then $\beta(\rho) = U \rho U^*$ for some unitary U .

What is the meaning of irreversibility?

Classical Mechanics: Newton's equation \implies Boltzmann equations

Boltzmann entropy $H(f) = -\int f \log f$.

Quantum mechanics Schrödinger equation \implies reduced evolution.

von Neumann entropy $S(\rho) = -\text{tr}(\rho \log \rho)$.

Properties of $S(\rho)$. 1) $\rho = P_\psi$ pure state $\implies S(\rho) = 0$

2) $S(U\rho U^{-1}) = S(\rho)$

3) For $\lambda_j \geq 0, \sum \lambda_j = 1$,

$$S\left(\sum_{\lambda_j} \lambda_j \rho_j\right) \geq \sum_{\lambda_j} S(\rho_j) \quad (54)$$

(due to concavity of \log)

4) (Entropy of measurement) If $P_M = \{\text{tr}(M_x \rho)\}$, where M_x is a positive operator-valued measure (POVM), then

$$H(P_M) \geq S(\rho) \quad (55)$$

with equality when M_x and ρ commute. (Measurement increases entropy (randomness) and more so, more 'non-commuting' M_x and ρ are.)

5) (Entropy of preparation) $H(P) \geq S(\rho)$ where $\rho = \sum p_x P_{\varphi_x}$ and $=$ iff $\{\varphi_x\}$ are orthogonal.

However, there is no H -theorem for $S(\rho)$, i.e in general $S(\rho)$ does not decrease (or increase) under the evolution. We look for a more general object which has monotonicity properties \implies relative entropy:

$$S(\rho_1, \rho_2) = \text{Tr}(\rho_1(\log \rho_1 - \log \rho_2)), \quad (56)$$

if $\overline{\text{Ran}}\rho_1 = \overline{\text{Ran}}\rho_2$ and ∞ otherwise.

Theorem 12. (Generalized H-theorem (Lindblad)) If β is a dynamical map then

$$S(\beta(\rho_1), \beta(\rho_2)) \leq S(\rho_1, \rho_2). \quad (57)$$

Note: if $\beta(\rho) = U\rho U^*$, where U is unitary, then

$$S(\beta(\rho_1), \beta(\rho_2)) = S(\rho_1, \rho_2). \quad (58)$$

14. WIGNER TRANSFORMATION

We introduce the following transformation of density matrices

$$\rho \rightarrow W_\rho(y, k),$$

where

$$W_\rho(y, k) := (2\pi\hbar)^{-\frac{d}{2}} \text{Tr}(T_{2y, k} I \rho)$$

where the operators $T_{y, k}$ and I can be defined as

$$T_{y, k} = e^{-i(kx+yp)/\hbar} \quad (59)$$

and

$$I : \psi(x) \rightarrow \psi(-x). \quad (60)$$

Thus the Wigner transform maps density matrices (quantum statistical states) into functions of the classical phase space which look like chemical statistical states.

Properties of Wigner transformation:

1) W_ρ is real;

2) $\int dk W_\rho(y, k) = \rho(y, y)$ (probability density in y);

3) $\int dy W_\rho(y, k) = \hat{\rho}(k, k)$ probability distribution in ρ , where recall that $\hat{\rho}(k, k')$ is the Fourier transform of $\rho(x, x')$;

4) $\rho_1 = \text{Tr}_2(\rho) \implies W_{\rho_1}(y_1, k_1) = \int dy_2 dk_2 W_\rho(y_1, y_2, k_1, k_2)$.

5) $i\hbar \frac{\partial \rho}{\partial t} = [H, \rho] \implies \partial_t W_\rho = -\{h, W_\rho\} + O(\hbar \nabla_k^2 W_\rho)$. where

$$\{a, b\} = \sum_{j=1}^n (\partial_{y_j} a \partial_{k_j} b - \partial_{y_j} b \partial_{k_j} a). \quad (61)$$

Compare this with the classical Liouville equation of Statistical Physics:

$$\partial_t w = -\{h, w\} \quad (62)$$

Before proving these statements we find an explicit form of W_ρ . To this end we use the Baker-Campbell-Hausdorff formula:

$$e^{-\frac{ikx}{\hbar}} e^{-\frac{iyp}{\hbar}} = e^{-i\frac{(kx+yp)}{\hbar}} e^{-i\frac{yk}{2\hbar}}. \quad (63)$$

More generally

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]} \quad (64)$$

if $[A, B]$ is a multiple of the identity. To check this compute

$$\partial_s(e^{sA} e^{sB}) = (A + e^{sA} B e^{-sA}) e^{sA} e^{sB} = (A + B + \int_0^s dr e^{rA} [A, B] e^{-rA}) e^{sA} e^{sB} = (A + B + s[A, B]) e^{sA} e^{sB}. \quad (65)$$

Using (63) we obtain that

$$W_\rho(y, k) = (2\pi\hbar)^{-\frac{d}{2}} e^{\frac{i y k}{\hbar}} Tr(B). \quad (66)$$

where

$$B = e^{-\frac{ikx}{\hbar}} e^{-i\frac{2yp}{\hbar}} I\rho. \quad (67)$$

Compute the integral kernel of B

$$B(x, x') = e^{-\frac{ikx}{\hbar}} \rho(-x + 2y, x'). \quad (68)$$

Hence

$$W_\rho(y, k) = (2\pi\hbar)^{-\frac{d}{2}} \int e^{-\frac{ik(x-y)}{\hbar}} \rho(2y-x, x) dx = (2\pi\hbar)^{-\frac{d}{2}} \int e^{-\frac{ik(x-y)}{\hbar}} \rho(y-(x-y), y+(x-y)) dx. \quad (69)$$

Therefore,

$$W_\rho(y, k) = (2\pi\hbar)^{-\frac{d}{2}} \int e^{-\frac{ikx}{\hbar}} \rho(y-x, y+x) dx. \quad (70)$$

HW: Prove 1), 3), 4). Hint for 1): use that $\rho(x, x') = \rho(x', x)$. Hint for 3): use that $x = \frac{1}{2}(x+y) + \frac{1}{2}(x-y)$. Hint for 4): follows from 3) and $yk = y_1 k_1 + y_2 k_2$, etc.

We show 2). We use that for nice functions f

$$(2\pi\hbar)^{-\frac{d}{2}} \int dk \hat{f}(k) = f(0). \quad (71)$$

Indeed, set $x = 0$ in $(2\pi\hbar)^{-\frac{d}{2}} \int dk e^{\frac{ixk}{\hbar}} \hat{f}(k) = f(x)$. Using this relation we obtain

$$\int dk W_\rho(y, k) = \rho(y-x, x+y)|_{x=0} = \rho(y, y). \quad (72)$$

Now we show 5). $W_{\frac{i}{\hbar}[H_0, \rho]}(y, k) = \frac{i}{\hbar} \frac{-\hbar^2}{2m} (2\pi\hbar)^{-\frac{d}{2}} \int (\partial_y^2 - \partial_{y'}^2) \rho(y-x, y'+x')|_{y'=y, x'=x} e^{\frac{ixk}{\hbar}} dx$

$$\begin{aligned} &= -\frac{i\hbar}{2m} \frac{1}{\hbar^{\frac{d}{2}}} \int (-\partial_y \partial_x - \partial_{y'} \partial_{x'}) \rho(y-x, y'+x')|_{x=x', y=y'} e^{\frac{ixk}{\hbar}} dx \\ &= -\frac{i\hbar}{2m} \frac{1}{\hbar^{\frac{d}{2}}} \int [(\partial_y \partial_{x'} + \partial_{y'} \partial_x) \rho + \frac{ik}{\hbar} (\partial_y + \partial_{y'}) \rho]|_{x'=x, y'=y} e^{\frac{ixk}{\hbar}} dx \\ &= -\frac{i\hbar}{2m} \frac{1}{\hbar^{\frac{d}{2}}} \int [(\partial_y \partial_{x'} + \partial_{y'} \partial_x) \rho|_{x'=x, y'=y} + \frac{ik}{\hbar} \partial_y \rho] e^{ixk} \hbar dx \\ &= \frac{k}{m} \partial_y \frac{1}{\hbar^{\frac{d}{2}}} \int \rho e^{ixk} \hbar dx = \frac{k}{m} \nabla_y W_\rho, \end{aligned} \quad (73)$$

where we used that $(\partial_y + \partial_{y'}) \rho|_{x'=x, y'=y} = \partial_y (\rho|_{x'=x, y'=y})$.

Furthermore, we have

$$\begin{aligned} W_{\frac{i}{\hbar}[V, \rho]}(y, k) &= \frac{i}{\hbar^2} \int (V(y - \frac{1}{2}x) - V(y + \frac{1}{2}x)) \rho e^{\frac{ixk}{\hbar}} dx \\ &= \frac{i}{\hbar^2} \int [-\nabla V(y)x + O(x^2)] \rho e^{\frac{ixk}{\hbar}} \end{aligned}$$

$$\begin{aligned}
 &= \frac{i}{\hbar^2} \int [-\nabla V(y)(-i\hbar\nabla_k) + O((\hbar\nabla)^2)]\rho \\
 &= (-\nabla V(y)\nabla_k + O(\hbar\nabla_k^2))W_\rho.
 \end{aligned} \tag{74}$$

Therefore, the equation

$$\frac{\partial \rho}{\partial t} = -\frac{i}{\hbar}[H, \rho] \tag{75}$$

implies

$$\partial_t W = \left(\frac{k}{m}\nabla_y - V(y)\nabla_k\right)W_\rho + O(\hbar)\nabla_k^2 W_\rho. \tag{76}$$

Let $h(y, k) = \frac{1}{2m}|k|^2 + V(y)$, and $\{F, G\} := \nabla_y F \nabla_k G - \nabla_k F \nabla_y G$, the Poisson Bracket. Then

$$\partial_t W_\rho = -\{h, W_\rho\} + O(\hbar\nabla_k^2 W_\rho). \tag{77}$$

The leading part is the classical Liouville equation:

$$\partial_t w = -\{h, w\} \tag{78}$$

Note that in Classical Mechanics it is obtained as

$$\partial_t w(y, k) = \partial_y w \dot{y} + \partial_k w \dot{k} = \partial_y w \partial_k h - \partial_k w \partial_y h \tag{79}$$

Thus, in the limit $\hbar \rightarrow 0$ the quantum statistics becomes classical statistics. This is confirmed by the following additional property

$$Tr(A\rho) = \iint a W_\rho dy dk,$$

where A is the Weyl quantization of $a(y, k)$:

$$A\psi(x) = \hbar^{-6} \iint \hat{a}(\xi, \eta) e^{i(\xi x + \eta p)/\hbar} d\xi d\eta, \tag{80}$$

where

$$a(y, k) = \hbar^{-6} \iint \hat{a}(\xi, \eta) e^{i(\xi y + \eta k)/\hbar} d\xi d\eta. \tag{81}$$

Note that this property implies an approximate the probability distribution in the phase space:

$$Prob(x \in \Omega, p' \in \Omega') \approx \int_\Omega \int_{\Omega'} W_\rho dy dk.$$

15. LECTURE 9. HARMONIC OSCILLATOR, PARTICLE IN AN EXTERNAL MAGNETIC FIELD, PERTURBATION THEORY

16. LECTURE 10. MANY-BODY SYSTEMS, ATOMS AND MOLECULES

17. LECTURE 11 (INDEPENDENT STUDY) HYDROGEN ATOM HAMILTONIAN, REVIEW OF HARMONIC OSCILLATOR AND PARTICLE IN AN EXTERNAL MAGNETIC FIELD