

Update: This Sunday December 13th the TA Ioannis Anapolitanos will hold office hours from 6 to 9. The office hours will take place at the Lounge of Mathematics Department. If none of the office hours works for you send an e-mail at ioannis.anapolitanos@utoronto.ca

Second update: The notes were updated today Sunday December 13th. Please make sure you read the updates.

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

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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. **Tests.** Undergraduates:

Midterm test October 21-29 (take home).

Final test Dec 14, 2009, 2:00-5:00pm, Location: SS2127

Graduates: The above plus a 20 min presentation.

Midterm and final exam will be on the material covered in the lectures.

The final exam will have 12 problems, 8 on the material covered in the midterm test and 4 on the material covered after the midterm test (the material covered after the midterm test: Quantum statistics and open systems, Specific examples, Perturbation theory, Many-body systems, The second quantization).

The 60% of the mark is due to the last 4 problems.

1.8. **Marking scheme.** Breakup of the grade:

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

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

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

1.10. **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*

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

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 operators 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 \rightarrow 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.

Wave Optics $\quad \rightarrow \quad$ Geometrical Optics

\downarrow

\downarrow

Quantum Mechanics $\quad \rightarrow \quad$ Classical Mechanics

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

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

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

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

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

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

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

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

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

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

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

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

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) $e^{-\frac{|x|^2}{2a\hbar^2}} \mapsto (\hbar a)^{d/2} e^{-\frac{a|k|^2}{2}}$ ($Re(a) > 0$). 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) $\sqrt{\frac{\pi}{2\hbar}} \frac{e^{-\sqrt{b/\hbar^2}|x|}}{|x|} \mapsto (|k|^2 + b)^{-1}$ ($b > 0, d = 3$). 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 $\psi, \phi \in C_0^\infty(\mathbb{R}^d)$.

$$(1) \quad -i\hbar \widehat{\nabla_x \psi}(k) = k \hat{\psi}(k).$$

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

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

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

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

$$(A \pm i)\psi = f \tag{12}$$

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

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

and therefore

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

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 $\text{Ran}(-i\hbar\partial_x - i) = L^2$. □

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

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

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

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

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 $K(\lambda)^T = V(H_0 + i\lambda)^{-1}$ (**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

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

(2) Prove that

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

(3)

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

(4)

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

6. CONSERVATION LAWS

We say that a physical quantity represented by an observable A is **conserved** if its average in any evolving state $\psi(t)$ is independent of t : $\forall \psi$

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

where $\psi = \psi(0)$ and $A(t) := e^{itH/\hbar} A e^{-itH/\hbar}$. If an observable A commutes with the Schrödinger operator H , i. e. $[A, H] = 0$, then the corresponding physical quantity is conserved. (**Homework.** Show this.) For example, since obviously $[H, H] = 0$, we 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:

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

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 $\sigma_{\text{ess}}(U^*AU) = \sigma_{\text{ess}}(A)$.

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

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

- (1) $\sigma_{\text{ess}}(H) = [0, \infty)$;
- (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 an orthogonal projection. Show that

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

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

Homework: If P is an orthogonal projection then $\text{Ran}P$ 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

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

is independent of the choice of basis.

Homework: Show the following properties of trace:

- 1) $\text{Tr}(\alpha A + \beta B) = \alpha\text{Tr}A + \beta\text{Tr}B$.
- 2) If A is a bounded and B is a trace class operator, then $\text{Tr}(AB) = \text{Tr}(BA)$.
- 3) $\text{Tr}A^* = \overline{\text{Tr}A}$
- 4) If $K\psi(x) = \int K(x, y)\psi(y)dy$, then $\text{Tr}K = \int K(x, x)dx$.

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

Homework: Let $\rho = \sum_{n=1}^\infty p_n P_{\psi_n}$, where $p_n \geq 0$ and $\sum p_n = 1$. Show that $\rho \geq 0$, $\text{Tr}\rho = 1$ 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

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

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

$$\|A\| \leq \text{Tr}|A| \quad (35)$$

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

Distance: $\|A - B\|_1, d_F(A, B) = \min\{\|\Psi - \Phi\| | \text{Tr}_{\text{envir}}P_\psi = A, \text{Tr}_{\text{envir}}P_\phi = B\}$.

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 $\rho = Tr_{envir}R$, which is given in terms of the partial trace Tr_{envir} 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

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

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

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

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

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

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

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

acting on $L^2(dxdy)$. 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 $U := e^{-i\frac{H_{tot}t}{\hbar}}$ 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

$$\begin{aligned} & \langle V_{ij} \phi, \psi \rangle_s = \langle \phi, V_{ij}^* \psi \rangle_s = \sqrt{\lambda_j} \langle \phi, \langle \chi_j, U^* \psi \chi_i \rangle_{en} \rangle_s \\ &= \sqrt{\lambda_j} \langle U \phi \chi_j, \psi \chi_i \rangle = \langle \sqrt{\lambda_j} \langle U \phi \chi_j, \chi_i \rangle_{en}, \psi \rangle_s \\ &\implies V_{ij} \phi = \sqrt{\lambda_j} \langle \chi_i, U \phi \chi_j \rangle_{en} \\ &\implies \sum_{i,j} V_{ij}^* V_{ij} \phi = \sum_{i,j} V_{ij}^* \sqrt{\lambda_j} \langle \chi_i, U \phi \chi_j \rangle_{en} \\ &= \sum_{ij} \lambda_j \langle \chi_j, U^* \langle \chi_i, U \phi \chi_j \rangle_{en} \chi_i \rangle_{en}. \\ &= \sum_j \lambda_j \langle \chi_j, U^* \sum_i \langle \chi_i, U \phi \chi_j \rangle_{en} \chi_i \rangle_{en} \\ &= \sum_j \lambda_j \langle \chi_j, U^* U \phi \chi_j \rangle_{en} = \sum_j \lambda_j \langle \chi_j, \phi \chi_j \rangle_{en} \\ &= \sum_j \lambda_j \phi = \phi \end{aligned} \quad (46)$$

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

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

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

For a Markov dissipative evolution β_t we define the generator by

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

so that

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

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

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

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:

$$\langle \rho, A \rangle = Tr_{syst}(A\rho). \tag{49}$$

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 $V \in B(\mathcal{H}_s)$,

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

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 $\exists \Phi : operators \rightarrow operators$, one-to-one and onto, such that

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

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 $S(\rho) = -tr(\rho \log \rho)$.

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

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

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

$$S(\sum \lambda_j \rho_j) \geq \sum_{\lambda_j} S(\rho_j) \tag{54}$$

(due to concavity of \log)

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

$$H(P_M) \geq S(\rho) \tag{55}$$

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:

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

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

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

$$S(\beta(\rho_1), \beta(\rho_2)) \leq S(\rho_1, \rho_2). \tag{57}$$

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

$$S(\beta(\rho_1), \beta(\rho_2)) = S(\rho_1, \rho_2). \tag{58}$$

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

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

Hamiltonian of molecule with N electrons and M nuclei of charges eZ_j ($N = \sum Z_j$) where $-e$ is the electron charge:

$$H = \frac{1}{2m} \sum_{i=1}^N -\frac{\hbar^2}{2m} \Delta_{x_i} + \sum_{i=1}^M -\frac{\hbar^2}{2m_i} \Delta_{y_i} + V(x, y), \quad (59)$$

where m is the electron mass, m_i is the mass of the i -th nucleus and

$$V(x, y) = \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|x_i - x_j|} - \sum_{i,j} \frac{e^2 Z_j}{|x_i - y_j|} + \frac{1}{2} \sum_{i \neq j} \frac{e^2 Z_i Z_j}{|y_i - y_j|}. \quad (60)$$

If the nuclei are infinitely heavy, then the molecular Hamiltonian takes the form

$$H_{mol}(y) = \frac{1}{2m} \sum_{i=1}^N -\frac{\hbar^2}{2m} \Delta_{x_i} + V(x, y). \quad (61)$$

In the special case of an atom (a single nucleus), we have

$$H_{at} = \frac{1}{2m} \sum_{i=1}^N -\frac{\hbar^2}{2m} \Delta_{x_i} + V(x), \quad (62)$$

where $V(x) = \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|x_i - x_j|} - \sum_i \frac{e^2 Z}{|x_i|}$ (assuming that the nucleus of the atom is at the origin).

Electrons are indistinguishable (purely quantum phenomenon)

$\implies |\Psi(x_1, \dots, x_N)|^2$ is symmetric w.r.t permutations of electron coordinates

$\implies \Psi$ is multiplied by ± 1 when a pair of coordinates are interchanged.

In fact electrons are Fermions which implies a more refined symmetry condition.

15.1. Spectra of atoms and molecules. Let H_n be the Schrödinger Operator of an atom with n electrons, in a center-of-mass frame. We have

Theorem 13. (*HVZ theorem*) $\sigma_{ess}(H_n) = [\Sigma_n, \infty)$ where $\Sigma_n = \inf \sigma(H_{n-1})$ (called the ionization threshold).

To obtain $\sigma_{ess}(H_n)$ we take one of the electrons to infinity and let it move freely there. The rest of the atom is placed in the ground state, so that the energy of the atom is

$$Energy = \Sigma_n + \frac{1}{2m} |k|^2 \quad \forall k \quad (63)$$

where k is the momentum of the electron which is placed at infinity.

What about the stability of atoms?

Show that H_n has at least one bound state. Let $\Psi_n(x_1, x_2, \dots, x_n)$ be the ground state of H_n . Assume for simplicity that the nuclear mass = ∞ and that for any n the one-electron density

$$\rho_n(x) := \int |\Psi_n(x, x_2, \dots, x_n)| dx_2 \dots dx_n$$

is spherically symmetric. We use the variational principle with the test function

$$\phi = \Psi_{n-1}(x_1, \dots, x_{n-1}) f(x_n), \quad (64)$$

where for simplicity we take a non-symmetric ϕ . Using that

$$H_n = H_{n-1} - \frac{\hbar^2}{2m} \Delta_{x_n} + I, \quad (65)$$

with

$$I := \sum_{i=1}^{n-1} \frac{e^2}{|x_i - x_n|} - \frac{e^2 Z}{|x_n|},$$

and using that

$$H_{n-1} \Psi_{n-1} = E_{n-1} \Psi_{n-1},$$

we obtain

$$H_n \phi = (E_{n-1} + I)\phi + \Psi_{n-1} \left(-\frac{\hbar^2}{2m} \Delta_{x_n} f \right).$$

This implies that

$$\langle H_n \rangle_\phi = E_{n-1} + \langle f, \left(-\frac{\hbar^2}{2m} \Delta + W \right) f \rangle,$$

where

$$\begin{aligned} W(x_n) &= \int \overline{\Psi_{n-1}}(x_1, \dots, x_{n-1}) I \Psi_{n-1}(x_1, \dots, x_{n-1}) d^{n-1}x \\ &= (n-1)e^2 \int \frac{\rho_{n-1}(y)}{|x-x_n|} dy - \frac{e^2 Z}{|x_n|}, \end{aligned}$$

where $\rho_{n-1}(x_1) = \int |\Psi_{n-1}|^2 dx_2 \dots dx_{n-1}$. Since ρ_{n-1} is spherically symmetric, we have by Newton's theorem

$$\int \frac{\rho_{n-1}(y) dy}{|y-x_n|} = \frac{1}{|x_n|} \int_{|y| \leq |x_n|} \rho_{n-1}(y) dy \leq \frac{1}{|x_n|} \int_{|y| < \infty} \rho_{n-1}(y) dy = \frac{1}{|x_n|}, \quad (66)$$

where we used that $\int \rho_{n-1}(y) dy = 1$. (Moreover, $\rho_{n-1}(x) = O(e^{-\delta|x|}) \implies \int_{|y| \leq |x_n|} \rho_{n-1}(y) dy = 1 + O(e^{-\delta|x_n|})$.) Hence

$$W(x_n) \leq \frac{(n-1)e^2}{|x_n|} - \frac{e^2 Z}{|x_n|} \stackrel{n=Z}{=} -\frac{e^2}{|x_n|}.$$

If f is an eigenfunction of the Hamiltonian with eigenvalue $-e_m$, then

$$\langle H_n \rangle_\phi \leq E_{n-1} + \langle f, \left(-\frac{\hbar^2}{2m} \Delta - \frac{e^2}{|x_n|} \right) f \rangle = E_{n-1} - e_m < E_{n-1}.$$

Remark. The Fechbach-Schur method with $P = |\phi\rangle\langle\phi|$ gives a more precise result: λ eigenvalue of H_n if $\lambda = E_{n-1} - e_m - U(\lambda)$ where

$$U(\lambda) = \langle IP^\perp (H_n^\perp - \lambda)^{-1} P^\perp I \rangle_\phi \geq 0. \quad (67)$$

Since electrons are indistinguishable, the test function $\phi = \Psi_{n-1}(x_1, \dots, x_n) f(x_n)$ is inappropriate so we antisymmetrize this function to obtain

$$\phi := \frac{1}{\sqrt{n}} (\Psi_{n-1}(x_1, \dots, x_{n-1}) f(x_n) \pm \Psi_{n-1}(x_1, \dots, x_{n-2}, x_n) f(x_{n-1}) \pm \dots \pm \Psi_{n-1}(x_2, \dots, x_n) f(x_1)) = \sum_{j=1}^n \phi^{(j)}. \quad (68)$$

Choose f so that

$$|\langle \phi_i, \phi_j \rangle| \ll 1 \quad \text{and} \quad |\langle \phi_i, \left(-\frac{\hbar^2}{2m} \Delta_{x_j} + I^{(j)} \right) \phi_j \rangle| \ll 1 \quad \text{for } i \neq j, \quad (69)$$

where $I^{(j)} := \sum_{i:i \neq j} \frac{e^2}{|x_i - x_j|} - \frac{e^2 Z}{|x_j|}$. Namely we take $f_\alpha(x) = \alpha^{\frac{3}{2}} f(\alpha x)$ with $\|f\| = 1$. Then for $i \neq j$ we have

$$\begin{aligned} &|\langle \phi_i, \phi_j \rangle| \\ &\leq \frac{\alpha^3}{n} \sup |f|^2 \int |\overline{\Psi_{n-1}}(x_1, \dots, \hat{x}_i, \dots, x_n) \Psi_{n-1}(x_1, \dots, \hat{x}_j, \dots, x_n)| dx_1 \dots dx_n \\ &\leq \left(\int dx_{n-1} \left(\int |\Psi_{n-1}|^2 d^{n-2}x \right)^{\frac{1}{2}} \right)^2 \frac{\alpha^3}{n} \sup |f|^2 \end{aligned}$$

and, similarly,

$$|\langle \phi_i, \left(-\frac{\hbar^2}{2m} \Delta_{x_j} + I^{(j)} \right) \phi_j \rangle| \lesssim \frac{\alpha^3}{n} \quad \text{for } i \neq j.$$

By taking $\alpha \rightarrow 0$, the last two equations imply (69) and therefore

$$\begin{aligned} \langle H \rangle_\phi &\leq E_{n-1} + \left\langle -\frac{\hbar^2}{2m} \Delta_x - \frac{e^2}{|x|} \right\rangle_{f_\alpha} + O\left(\frac{\alpha^3 n^2}{n}\right) \\ &= E_{n-1} + \alpha^2 \left\langle -\frac{\hbar^2}{2m} \Delta \right\rangle_f - \alpha \left\langle \frac{e^2}{|x|} \right\rangle_f + O(\alpha^3 n) < E_{n-1} \end{aligned}$$

if $\alpha \ll \frac{1}{\sqrt{n}}$ and $\alpha < \frac{(-\frac{\hbar^2}{2m}\Delta)_f}{\langle \frac{\epsilon^2}{|x|} \rangle_f}$. This proves the existence of ground state energy for $H_n \forall n$.

Homework: Go over the proof above and, whenever necessary, fill in the details.

15.2. Atoms in a weak external field. Consider an atom in a weak external field (e.g. a weak laser or magnetic trap). Its Schrödinger operator is

$$H_{n\epsilon} = \sum_{i=1}^n \left(-\frac{\hbar^2}{2m} \Delta_{x_i} - \frac{e^2}{|x_j|} + \epsilon \tilde{W}(x_i) \right) + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|x_i - x_j|}. \quad (70)$$

If $\epsilon \tilde{W}$ is a trap (magnetic or optical), then $\tilde{W} \rightarrow \infty$ as $|x| \rightarrow \infty$. We assume $W \geq 0$. Here ϵ is a small positive number ($\epsilon \rightarrow 0$), called the coupling constant. Though ϵ is small, $\epsilon \tilde{W}$ could be very large for large $|x|$.

We want to find the leading order correction as $\epsilon \rightarrow 0$ to the ground state energy, $E_{n\epsilon}$, of the atom in the external potential above. We write

$$H_{n\epsilon} = H_n + \epsilon W, \text{ where } H_n := H_{n\epsilon=0} \text{ and } W(x) = \sum_i \tilde{W}(x_i). \quad (71)$$

Let Ψ_n be the ground state of H_n . Use Feshbach-Schur method with the projection $P = |\Psi_n\rangle\langle\Psi_n|$. Since P is a rank-1 projection, we have

$$E_{n\epsilon} \text{ is an eigenvalue of } H_{n\epsilon} \leftrightarrow E_{n\epsilon} \text{ solves the equation } f(\lambda) = 0,$$

where

$$f(\lambda) := \langle H_{n\epsilon} - \lambda \rangle_{\Psi_n} - \epsilon^2 U(\lambda),$$

with

$$U(\lambda) := \langle WP^\perp(H_{n\epsilon}^\perp - \lambda)P^\perp W \rangle_{\Psi_n},$$

and

$$H_{n\epsilon}^\perp = P^\perp H_{n\epsilon} P^\perp \text{ and } W(x) = \sum_i \tilde{W}(x_i).$$

Let E_n and E_n^\perp be the smallest eigenvalue (the ground state energy) and the second smallest eigenvalue of H_n . Assume

$$\epsilon \leq \frac{\frac{1}{2}(E_n^\perp - E_n)}{\langle W \rangle_{\Psi_n}}.$$

Compute

$$\langle H_{n\epsilon} - \lambda \rangle_{\Psi_n} = E_n + \epsilon \langle W \rangle_{\Psi_n}.$$

This implies

$$E_{n\epsilon} = E_n + \epsilon \langle W \rangle_{\Psi_n} - \epsilon^2 U(E_{n\epsilon}). \quad (72)$$

Estimate $U(E_{n\epsilon})$. Since $U(\lambda) \geq 0$, we have that $E_{n\epsilon} \leq E_n + \epsilon \langle W \rangle_{\Psi_n} \leq \frac{1}{2}(E_n^\perp - E_n)$. Hence

$$\begin{aligned} H_{n\epsilon}^\perp - E_{n\epsilon} &= H_n^\perp + \epsilon P^\perp W P^\perp - E_{n\epsilon} \geq H_n^\perp - E_{n\epsilon} \\ &\geq H_n^\perp - E_n - \frac{1}{2}(E_n^\perp - E_n) \geq E_n^\perp - E_n - \frac{1}{2}(E_n^\perp - E_n) \geq \frac{1}{2}(E_n^\perp - E_n). \end{aligned}$$

(In the inequality before the last one we used that E_n^\perp is the smallest eigenvalue of H_n^\perp and therefore $H_n^\perp \geq E_n^\perp$.)

This implies

$$U := \langle WP^\perp(H_{n\epsilon}^\perp - E_{n\epsilon})^{-1}P^\perp W \rangle_{\Psi_n} \leq (E_n^\perp - E_n)^{-1} \langle WP^\perp W \rangle_{\Psi_n} = (E_n^\perp - E_n)^{-1} \|P^\perp W \Psi_n\|^2 = C.$$

Thus U is uniformly bounded in ϵ . This and (72) imply that for $\epsilon \leq \frac{\frac{1}{2}(E_n^\perp - E_n)}{\langle W \rangle_{\Psi_n}}$,

$$E_{n\epsilon} = E_n + \epsilon \langle W \rangle_{\Psi_n} - O(\epsilon^2). \quad (73)$$

Homework. Redo carefully the proof for the special case of hydrogen atom.

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

17. LECTURE 12 2ND QUANTIZATION

It is sometimes convenient or necessary to allow the number of particles to fluctuate. Consider a system of n spinless Bosons with the Schrödinger operator

$$H_n = \sum_{i=1}^n -\frac{\hbar^2}{2m} \Delta_{x_i} + \frac{1}{2} \sum_{i \neq j} v(x_i - x_j), \quad (74)$$

where $v(x_i - x_j)$ are pair potentials (**always assumed to be real and bounded** unless we deal with atoms and molecules, in which case they are Coulomb) acting on the space

$$L^2_{symm}(\mathbb{R}^{3n}) = \{\Psi \in L^2(\mathbb{R}^{3n}) | \Psi \text{ is symmetric w.r.t permutations of coordinates } x_1, \dots, x_n \in \mathbb{R}^3\}.$$

We define a new Hilbert space

$$\mathcal{F}_{bos} := \bigoplus_{n=0}^{\infty} \mathcal{F}_n, \quad (75)$$

where $\mathcal{F}_0 = \mathbb{C}$, and $\mathcal{F}_n = L^2_{symm}(\mathbb{R}^{3n})$, $n \geq 1$. We equip this space with inner product

$$\langle \Psi, \Phi \rangle = \sum_{n=0}^{\infty} \int \overline{\Psi_n(x_1, \dots, x_n)} \Phi_n(x_1, \dots, x_n) d^n x, \quad (76)$$

where Ψ_n is the n -th component of Ψ (**in this section Ψ_n is an arbitrary function in \mathcal{F}_n , not just the ground state of H_n as in the previous section**). Then \mathcal{F}_{bos} becomes a Hilbert space. \mathcal{F} is called the *Bosonic Fock space*.

On \mathcal{F}_{bos} we define the operator

$$H = \bigoplus_{n=0}^{\infty} H_n, \quad (77)$$

where $H_0 = 0$ and H_n , $n \geq 1$, are as above.

Homework. Show that H is self-adjoint. (As mentioned above, the pair potentials, $v(x_i - x_j)$, are assumed to be real and bounded.)

The operator H is called the 2nd quantized Schrödinger operator. The reason for this name will become clear later. There is a special vector, $\Omega := (1, 0, 0, \dots) \in \mathcal{F}_{bos}$, in \mathcal{F}_{bos} , called the *vacuum vector*. Note that $H\Omega = 0$.

One of the advantages of the 2nd quantization is the representation of operators on the Fock space \mathcal{F}_{bos} in terms of creation and annihilation operators (raising and lowering the number of particles.) The annihilation operator is the operator valued distribution $f \rightarrow a(f)$ on \mathcal{F}_{bos} defined as

$$(a(f)\Psi)_n = \sqrt{n+1} \int \overline{f(x)} \Psi_{n+1}(x, x_1, \dots, x_n) dx \quad (78)$$

and $a(f)\Omega = 0$. Here $f \in L^2(\mathbb{R}^3)$. The creation operator $a^*(f)$ is the operator adjoint to $a(f) : a^*(f) = a(f)^*$. Find an explicit expression for $a^*(f)$:

$$\begin{aligned} \langle a(f)^* \Phi, \Psi \rangle &= \langle \Phi, a(f)\Psi \rangle = \sum_n \langle \Phi_n, (a(f)\Psi)_n \rangle \\ &= \sum_n \sqrt{n+1} \int dx_1 \dots dx_n dx \overline{\Phi_n(x_1, \dots, x_n)} f(x) \Psi_{n+1}(x, x_1, \dots, x_n) = \\ &\text{(relabel } x, x_1, \dots, x_n \rightarrow x_1, x_2, \dots, x_{n+1}) \\ &= \sum_n \sqrt{n+1} \int dx_1 \dots dx_{n+1} f(x_1) \overline{\Phi_n(x_2, \dots, x_{n+1})} \Psi_{n+1}(x_1, \dots, x_{n+1}) \end{aligned} \quad (79)$$

Note: we could have used any other relabeling e.g

$$x, x_1, \dots, x_n \rightarrow x_2, x_1, x_3, \dots, x_{n+1}, \text{ etc.}$$

Using these different relabelings, we obtain

$$\begin{aligned} \langle a(f)^* \Phi, \Psi \rangle &= \sum_n \sqrt{n+1} \int d^{n+1} x \frac{1}{n+1} (f(x_1) \Phi_n(x_2, \dots, x_{n+1}) + \dots + f(x_{n+1}) \Phi_n(x_1, \dots, x_n)) \Psi_{n+1}(x_1, \dots, x_{n+1}) \\ &\implies (a(f)^* \Phi)_{n+1} = \sqrt{n+1} S_{n+1}(f(x_1) \Phi_n(x_2, \dots, x_{n+1})), \end{aligned}$$

where S_n is the symmetrization operator for permutation of n indices on $L^2(\mathbb{R}^{3n})$. S_n is the orthogonal projection of $L^2(\mathbb{R}^{3n})$ to $L^2_{symm}(\mathbb{R}^{3n})$. (Other notation $S_{n+1}(f \otimes \Phi_n) = f \otimes \Phi_n$.)

Thus,

$$a(f) : 0 \oplus \dots \oplus \Psi_{n+1} \oplus 0 \dots \rightarrow 0 \oplus \dots \oplus \tilde{\Psi}_n \oplus 0 \dots \quad (80)$$

and

$$a^*(f) : 0 \oplus \dots \oplus \Psi_n \oplus 0 \dots \rightarrow 0 \oplus \dots \oplus \tilde{\Psi}_{n+1} \oplus 0 \dots \quad (81)$$

(We write elements of \mathcal{F}_{bos} as $\Psi = \bigoplus_{n=0}^{\infty} \Psi_n$.)

Homework: Show that

$$[a(f), a(g)] = \langle f, g \rangle, [a(f), a(g)] = [a^*(f), a^*(g)] = 0. \quad (82)$$

We write formally

$$a(f) = \int \overline{f(x)} a(x) dx, a^*(f) = \int f(x) a^*(x) dx, \quad (83)$$

and consider $a(x), a^*(x)$ as operator-valued distributions satisfying

$$[a(x), a^*(y)] = \delta(x - y), [a^\#(x), a^\#(y)] = 0. \quad (84)$$

We think of $a^\#(x)$ as $a^\#(x) = a^\#(\delta_x)$.

Consider the free Schrödinger operator: $H_0 = \bigoplus_{n=0}^{\infty} H_{0n}$ where $H_{0n} = \sum_{i=1}^n -\frac{\hbar^2}{2m} \Delta_{x_i}$ is the free n -particle Schrödinger operator ($V = 0$). We claim that

$$H_0 = \int a^*(x) \left(-\frac{\hbar^2}{2m} \Delta_x\right) a(x) dx. \quad (85)$$

Here, given an operator h acting on $L^2(\mathbb{R}^3)$, we think of $h_x a(x)$ as the result of the operator h acting on the parameter x , $h_x a(x) = \int h(x, y) a(y) dy$, where $h(x, y)$ is the integral kernel of h . The equation (85) is a formal expression which is rigorously understood as

$$H_0 = \sum_i a^*(f_i) \left(-\frac{\hbar^2}{2m} \Delta_{f_i}\right) a(f_i), \quad (86)$$

where $\{f_n\}$ is an orthonormal basis in $L^2(\mathbb{R}^3)$. The latter expression is obtained from the previous one by inserting formally the partition of unity $\sum_n |f_n\rangle \langle f_n|$ into the former expression. However, the former expression is much more convenient to work with which we take advantage of.

Proof. We prove formally that (85) gives $H_0 = \bigoplus_{n=0}^{\infty} H_{0n}$.

$$\begin{aligned} (H_0 \phi)_n &= \sqrt{n} \frac{1}{n} \int dx [\delta(x_1 - x) \left(-\frac{\hbar^2}{2m} \Delta_x \Phi\right)(x_2, \dots, x_n) + \dots + \delta(x_n - x) \left(-\frac{\hbar^2}{2m} \Delta_x a(x) \Phi\right)_{n-1}(x_1, \dots, x_{n-1})] \\ &\quad - \frac{1}{\sqrt{n}} \int dx [\delta(x_1 - x) \frac{\hbar^2}{2m} \Delta_x \sqrt{n} \Phi_n(x, x_1, \dots, x_{n-1}) + \dots + \delta(x_n - x) \Delta_x \sqrt{n} \Phi_n(x_1, \dots, x_{n-1}, x)] \\ &= - \sum_{i=1}^n \frac{\hbar^2}{2m} \Delta_{x_i} \Phi_n(x_1, \dots, x_n) \end{aligned} \quad (87)$$

as claimed. \square

Let

$$V = \frac{1}{2} \int a^*(x) a^*(y) v(x - y) a(x) a(y) dx dy.$$

(V annihilates particles at x and y and the creates particles at x and y .)

Homework: Show that

$$(V \Phi)_n = \frac{1}{2} \sum_{i \neq j} v(x_i - x_j) \Phi_n(x_1, \dots, x_n). \quad (88)$$

We define the operators $N = \bigoplus_{n=0}^{\infty} n$ and $P = \bigoplus_{n=0}^{\infty} P_n$ where $P_n = \sum_{j=1}^n p_j$, which are called the *number operator* and *momentum operator*, respectively.

Remark. Instead of fixing the number of particles, i.e working on the eigenspace $\{N = n\}$ we can fix the average number of particles:

$$\langle \Psi, N \Psi \rangle = n \text{ in a state } \Psi. \quad (89)$$

Homework: Show that

- 1) $N = \int a^*(x)a(x)dx$
- 2) $P = \int a^*(x)(-i\hbar\nabla_x)a(x)dx$
- 3) $[H_0, N] = 0 = [H_0, P]$
- 4) $[V, N] = 0 = [V, P]$ and $[H, N] = 0 = [H, P]$.

The equations $[H, N] = 0$ and $[H, P] = 0$ imply the **conservation of the particle number and total momentum**. We prove $[H_0, P] = 0$:

$$\begin{aligned} [H_0, P] &= \left[\int dx a^*(x) \left(-\frac{\hbar^2}{2m} \Delta_x \right) a(x), \int dy a^*(y) (-i\hbar \nabla_y) a(y) \right] \\ &= \int \int dx dy a^*(x) \left(-\frac{\hbar^2}{2} \Delta_x \right) [a(x), a^*(y)] (-i\hbar \nabla_y) a(y) + \int \int a^*(y) (-i\hbar \nabla_y) [a(x), a^*(y)] (-i\hbar \Delta_x) a(x) \\ &= \int dx a^*(x) \left[-\frac{\hbar^2}{2m} \Delta, -i\hbar \nabla \right] a(x) = 0, \end{aligned}$$

where in the last step we used that $[a(x), a^*(y)] = \delta(x - y)$.

Homework: Show that

$$[a^*(x) \Delta_x a(x), a(y)] = [a^*(x), a(y)] \Delta_x a(x).$$

Proposition 14. Any $\Phi = \oplus \Phi_n$ can be written as

$$\Phi = \sum_n \frac{1}{\sqrt{n!}} \int \Phi_n(x_1, \dots, x_n) \prod_{j=1}^n a^*(x_j) \Omega d^n x. \quad (90)$$

Proof. Using the definition we compute

$$(a^*(y_1) \Omega)_n = \sqrt{1} S_1(\delta(x_1 - y_1)) \delta_{n,1}$$

and

$$(a^*(y_2) a^*(y_1) \Omega)_n = \sqrt{2} S_2(\delta(x_1 - y_1) \delta(x_2 - y_2)) \delta_{n,2}.$$

Homework: Show by induction that

$$(a^*(y_n) \dots a^*(y_1) \Omega)_m = \sqrt{n!} S_n \left(\prod_{j=1}^n \delta(x_j - y_j) \right) \delta_{n,m}. \quad (91)$$

The last equation implies that

$$\frac{1}{\sqrt{n!}} \int \Phi_n(y_1, \dots, y_n) \prod a^*(y_j) \Omega d^n y = S_n \Phi_n(x_1, \dots, x_n), \quad (92)$$

which implies the statement of the proposition. \square

We now prove (88). Let

$$\Phi_n = \frac{1}{\sqrt{n!}} \int \Phi_n(x_1, \dots, x_n) \prod a^*(x_j) \Omega d^n x. \quad (93)$$

Recall that $V \Phi_n = \frac{1}{\sqrt{n!}} \int \int dx dy d^n x a^*(x) a^*(y) v(x-y) a(x) a(y) \Phi_n(x_1, \dots, x_n) \prod a^*(x_j) \Omega$. Pull $a(y)$ through $\prod_{j=1}^n a^*(x_k)$:

$$a(y) \prod_{i=1}^n a^*(x_j) \Omega = \sum_{i=1}^n \delta(y - x_i) \prod_{k \neq i} a^*(x_k) \Omega. \quad (94)$$

Therefore,

$$\begin{aligned} V \Phi_n &= \frac{1}{\sqrt{n!}} \int \int dx dy d^n x a^*(x) a^*(y) v(x-y) \Phi_n(x_1, \dots, x_n) a(x) \sum_{i=1}^n \delta(y - x_i) \prod_{k \neq i} a^*(x_k) \Omega \\ &\stackrel{\text{Pull } a(x)}{=} \frac{1}{\sqrt{n!}} \int \int dx dy d^n x a^*(x) a^*(y) v(x-y) \Phi_n(x_1, \dots, x_n) \sum_{i=1}^n \delta(y - x_i) \sum_{j \neq i} \delta(x - x_j) \prod_{i=1}^n a^*(x_k) \Omega \\ &= \frac{1}{\sqrt{n!}} \sum_{i=1}^n \sum_{j \neq i} v(x_i - x_j) \Phi_n(x_1, \dots, x_n) \prod_{i=1}^n a^*(x_k) \Omega. \end{aligned}$$

Consider the Heisenberg evolution of $a(x)$:

$$a(x, t) = e^{\frac{iHt}{\hbar}} a(x) e^{-\frac{iHt}{\hbar}}.$$

Homework. Show that $a(x, t)$ satisfies the differential equation

$$i\hbar \frac{\partial}{\partial t} a(x, t) = -\frac{\hbar^2}{2m} \Delta_x a(x, t) + \int dy v(x-y) a^*(y, t) a(y, t) a(x, t). \quad (95)$$

This is an operator Hartree equation. Hint: Use that $a(x, t)$ satisfies the Heisenberg equation:

$$i\hbar \frac{\partial}{\partial t} a(x, t) = -[H, a(x, t)]. \quad (96)$$

and compute the commutator $[H, a(x, t)] = e^{\frac{iHt}{\hbar}} [H, a(x)] e^{-\frac{iHt}{\hbar}}$.