J Theory of Operators: II

1. Representing operators

(a) Earlier in the class we spoke about how we could “represent” vectors. That is any vector can be represented as a linear combination of a complete set of vectors. (If this statement is not clear, please revise Section D and also look through the Pauli Spin matrix homework and handout where we learnt how to represent the spin operators using the kets $|SG^+_2⟩$ and $|SG^-_2⟩$.)

(b) Operators can be represented in a similar for. In fact if you have a complete set of vectors $\{ |i⟩ \}$, we can write an operator as a matrix. What we mean by this is we could represent an operator using a collection of matrix elements that have the following form:

$$A_{j,l} \equiv ⟨j | \hat{A} | l⟩ \quad (J.1)$$

$A_{j,l}$ is the $(j, l)$-th element of the matrix that is used to represent the operator $\hat{A}$. (Make sure to compare this with the Pauli spin matrix homework so you understand what’s going on clearly.)

(c) Does this definition make sense? $\hat{A} |l⟩$ is another vector. You could call it $|m⟩$ if you like. In that case the right hand side of Eq. (J.1) is the “dot” product of two vectors: $⟨j |$ and $|m⟩$. The “dot” product of two vectors is a number. Hence the definition in Eq. (J.1) makes sense. (If these arguments are not a 100% clear to you, you need to go back and revise Section D and the related appendix.)

(d) For Eq. (J.1) to be useful we should know what $\hat{A}$ does to $|l⟩$ when it acts on it.

2. Let’s now consider the individual parts of the Hamiltonian as seen in the description of the time-dependent and time-independent Schrödinger Equation. Here we will discuss representations for the Hamiltonian.

(a) The kinetic energy operator for the Hamiltonian is the second derivative operator. What we really did before we obtained the differential equation for the time-independent Schrödinger Equation for the particle in a box case is the following:

$$H |ψ⟩ = E |ψ⟩ \quad (J.2)$$

(b) We wrote this equation in the coordinate representation:

$$H \int dx \langle x | ψ \rangle = E |ψ⟩$$

$$\langle x' | K + V \int dx \langle x | ψ \rangle = E \langle x' | ψ⟩ \quad (J.3)$$

$$\int dx \langle x' | K | x⟩ \langle x | ψ⟩ + \int dx \langle x' | V | x⟩ \langle x | ψ⟩ = Eψ(x') \quad (J.4)$$
Note we have used the definition: \( \psi(x') \equiv \langle x' | \psi \rangle \) in the last equation above.

(c) Here we did something but never spoke about it. We implicitly made the assumption that

\[ \langle x' | V | x \rangle = V(x) \delta_{x,x'} . \]  

That is the potential energy does not depend on two points in space but only depends on one point.

(d) Does this make sense? The classical definition of the potential energy is the energy due to the position of an object and hence it should depend only on one index \( x \) which is the position of the object. Such potential energies are called \textit{local} potential energies. There exists a family of potential energies where we cannot make this simplification, that is we have to leave \( V \) as a function of two points as in the equation above and these are call \textit{non-local} potentials. We will not see any \textit{non-local} potentials in this course.

(e) This assumption of local potentials reduced our equation to:

\[ \int dx \langle x' | K | x \rangle \langle x | \psi \rangle + V(x) \psi(x) = E \psi(x') \]  

The first on the left hand side is another way to write the second derivative operator and this is how we got our differential equation that we solved for the particle in a box and other one-dimensional problems.

(f) The reason we are going through this digression is to realize that the matrix element of the operator we defined in Eq. (1.12) is something we implicitly used in writing down the differential equation. The differential equation had the corresponding form only because we chose to write the equation in the coordinate representation!! (We could have chosen any other complete set to write the Schrödinger Equation in and in such a case we would have needed the matrix elements in that basis set.)