What we learned so far by doing QM

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Answers given below are basic guides, and you are asked to provide your own answers, when the guide is simply that and does not give the final answer explicitly.

1. Time dependent Schrödinger equation (SE) for a non-relativistic particle
   (a) What is it? Why is deterministic? $i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \hat{H}\Psi(x,t)$. This is deterministic, since knowing $\Psi(x,t=0)$ (or any other fixed time) we know $\Psi(x,t)$ at any other time. [Further reading: L2 page 1, ...]
   (b) What are its general solutions?
      i. Case of quantized/bound state solutions (like parrticle in a box, harmonic oscillator): $\Psi(x,t) = \sum_n c_n\psi_n(x)\exp(-iE_nt/\hbar)$ where $c_n = \int dx\psi_n(t)^*\Psi(x,t=0)$. Here, $\psi_n(x)$ is the stationary state solution normalized to $\int dx\psi_m^*\psi_n = \delta_{m,n}$. [See 7, below]
      ii. Case of continuum/scattering state solutions (like free electron case): We covered the free electron case. In that case, $\Psi(x,t) = \int dk\phi(k)\psi_k(x)\exp(-iE_kt/\hbar)$ where $\phi(k) = \int dx\psi_k(x)^*\Psi(x,t=0)$. $\psi_k(x) = \frac{\exp(ikx)}{\sqrt{2\pi}}$. The plane wave statioinary state $\psi_k(x)$ was "normalized" so that $\int dx\psi_k^*\psi_l = \delta(k-l)$. [See 7, below]

2. What is the meaning of $\Psi(x,t)$? What is $\rho(x,t)$ and $j(x,t)$? What is the measning of c_n (particle in a box, harmonic oscillator)? How about $\phi(k)$ (free electron case)? How does the measurement affect $\Psi(x,t)$? Can you (sort of) write down the wave function right after the measurement, knowing what the result is? $\Psi(x,t)$ is the probability amplitude. $\rho(x,t) = |\Psi|^2$ is the probability density function. ρdx give the probability that the measurement of the particle position will fall within $[x, x+dx]$ (or $[x-dx/2, x+dx/2]$ or similar). $j(x,t) = Re(-\frac{1}{m}i\hbar\Psi^*\frac{\partial}{\partial x}\Psi)$ is the "probability flux." c_n and $\phi(k)$ are all probability amplitudes, just like $\Psi(x,t)$. The difference is that $|c_n|^2$ is the probability that the measurement will pick the state $\psi_n(x)$ while $|\phi(k)|^2dk$ is the probability that the measurement will pick a state that consists of states $\psi_l(x)$ with l centered at k and width dk (wave packet!). The measurement process affects $\Psi(x,t)$ dramatically -- it suddenly defines a new wave function, which the old wave function changes ("collapses") to. In the case of c_n, the wave function after the measurement is very simple: $\psi_n(x)$ (stationary state -- energy eigen state). Important points to remember here are that (1) wave function should be normalized after the measurement (particle does not go anywhere) and (2) there is an ambiguity in the overall phase factor ("de-coherence" in the measurement process). In the case of the measurement of position $\Psi(x,t)$ or wave vector $\phi(k)$, the wave function after the measurement is a wave packet, whose shape will be dependent on the measurment tool (this is why I say "sort of"). [Futher reading: Quiz 2, L1 pages 5,6, HW 1.2 (prob 1.14), L2 page 2, L4 page 10, ...]

3. Probability sum rule and particle conservation – what are they, and when do they hold? What constraint(s) do they put on $\Psi(x,t)$? `Probability sum rule simply means` $\sum Probability = 1$ `or` $\int Probability = 1$. `For,` $\Psi(x,t)$, c_n, $\phi(k)$, `it means` $\int dx|\Psi(x,t)|^2 = 1$, $\sum_n |c_n|^2 = 1$, `and` $\int dk|\phi(k)|^2 = 1$. `The time independence implied in` $\int dx|\Psi(x,t)|^2 = 1$ `can be called the "particle conservation," which holds when the potential is not complex.` $\Psi(x,t) \to 0$ `when` $x \to 0$, `as well as its derivatives. [Futher reading: L2 page 8, HW 2.1 (prob 1.15), L4 page 10, L6 page 6, ...]`

4. What are the intuitive/qualitative meanings of $\langle\hat{x}\rangle$ and Δx? What are the mathematical definitions? What are the useful things to remember when one calculates $\langle\hat{x}\rangle$, Δx, $\langle\hat{p}\rangle$ and Δp? $\langle\hat{x}\rangle$ `= Mean position,` Δx `= width in position.` $\langle\hat{O}\rangle \equiv \int dx \Psi(x,t)^* \hat{O} \Psi(x,t)$, `and` $\Delta O = \sqrt{\langle(\hat{O} - \langle\hat{O}\rangle)^2\rangle = \langle\hat{O}^2\rangle - \langle\hat{O}\rangle^2}$. `Parity consideration is often useful for figuring out these quantities. For` $\langle\hat{p}\rangle$ `or` Δp, `note that the mean position of the wave function is of no importance. Also, note that` $\langle\hat{p}^2\rangle$ `is proportional to the kinetic energy. This is often useful. [HW 2.3 (prob 2.17), Quiz 3, HW 2.5, prob. 2.4, ...]`

5. What is the qualitative meaning of the Heisenberg Uncertainty Principle $\Delta x \Delta p \geq \hbar/2$? Or, more loosely put without losing any physical meaning, $\Delta x \Delta p \gtrsim \hbar$. Can you put this into the $\Delta x \Delta k$ form? Can you explain what it means to a "lay photographer" who has some understanding of waves and Fourier analysis? `The qualitative meaning is that if you specify the wave length accurately the position of the wave is ill defined, and if you define the position of the wave (narrow wave packet) then the wave length of the wave is ill defined.` $\Delta x \Delta k \sim 1$. `To a lay person who knows Fourier analysis, one could say "well ... if you take a photograph (two dimensional intensity map), fourier transform it, make it sharp in the fourier space, and then do an inverse fourier transform -- what do you find?" Hopefully he will say, "the image becomes blurry." Then, you could say, "see .. that is the HUP, except that we are talking about matter waves in the case of the HUP, not the wavy pattern of a photograph." [H1.3, L3 page 4, L6 page 7 (note some new note there), ...]`

6. Time independent Schrödinger equation (TISE)

   (a) What is it? How *does* the solution evolve in time? $\hat{H}\psi(x) = E\psi(x)$. `The solution evolves in time as` $\psi(x)\exp(-iEt/\hbar)$. `[L3 page 9, ...]`

   (b) How come it is so useful? Or, how can one go from here to the solutoin of the full Time dependent Schrödinger Equation? `Because of the linearity of the SE, and the completeness of stationary states (see 7 below). [L4 page 7, ...]`

7. Stationary state, with quantized or continuum energies

   (a) What is it? Why is it called a stationary state? `Solution of TISE. Energy eigen state. Because the expectation value of` *`any`* `operator` $\langle\hat{O}\rangle$ `is a constant in time for a stationary state [as long as` $\hat{O}$ `does not have any explicit time dependence itself.]` $\hat{O} = 1, \hat{x}, \hat{p}, \hat{x}^2, \hat{p}^2$ `etc., for example. [L3 page 10, and lecture, ...]`

   (b) Ortho-normality relationship? $\int dx \psi_m^* \psi_n = \delta_{mn}$ `for quantized cases, and` $\int dk \psi_k^* \psi_l = \delta(k-l)$ `for continuum cases (we saw only one case -- free particle -- so far, but that is ok). [L4 page 7, L5 page 8, L6 page 4, ...]`

(c) How do you get *non-stationary* states and what governs the time dependence? Non-stationary states are obtained by mixing (that is, forming linear combinations of) stationary states. Time dependence of $\langle \hat{O} \rangle$ is given by angular frequencies, which are differences in energies of involved stationary states divided by $\hbar$. [L3 page 11, L4 pages 12,13, prob 2.5, ...]

(d) The implication of the "completeness"? Any physical wave function $f(x)$ can be written as $\sum_n c_n \psi_n$ or $\int dk \phi(k) \psi_k$ where ψ_n and ψ_k are stationary states in the case of quantized and continuum energies, respectively. Then, each term evolves in time according to E_n or E_k (see 1b above). [L4 page 7, L5 page 8, L6 page 4, ...]

(e) By now, do you have a "gut sense" of why $E > \min(V(x))$ (I mean aside from the cryptic solution of the note)? See if you can make a qualitative connection from HW 3.2 (Prob 2.3) to this question. [This problem moved from 14 below.]

8. General boundary conditions for stationary state $\psi(x)$ and its derivative $\psi'(x)$? ψ is always continuous. ψ' can be discontinuous if potential is infinite. Note that boundary conditions for the total wave function $\Psi(x,t)$ is more relaxed, namely $\Psi(x,t)$ can be discontinous, although such case is often a pathetic mathematical example, almost always. [HW 4.4 (prob 2.42), L4 pages 4,5, L6 page 7 (note), ...]

9. Infinite square well or "particle in a box" [L4!]

   (a) Can you quickly derive eigenstates and eigenvalues, possibly with a little bit of help from your note? Your answer should be "Yes!!"

   (b) Do you know parity properties of stationary states? From ground state, e-o-e-o-...

   (c) Can you work out the general solution for the SE in this case for a given initial condition $\Psi(x,0)$? Assuming you got ortho-normalized ψ_n, proceeding like in 1.b.i is the standard way. Sometimes trigonometric identity can give you a short-cut, as in Quiz 4.2. [HW 3.4 (prob 2.37), HW 3.4 (prob 2.38), ...]

10. Linear operators and their commutator – do you know their definitions and simple properties? What is $\hat{p}$? $\hat{O}(a\psi_1 + b\psi_2) = a\hat{O}\psi_1 + b\hat{O}\psi_2$. $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$. ... $\hat{p} = -i\hbar\frac{\partial}{\partial x}$. [L5 page 2, L3 pages 1,2, HW 3.1, Quiz 4.1, ...]

11. Harmonic oscillator [L5!]

    (a) What is the Hamiltonian? $\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$

    (b) Can you go back and forth between the $(\hat{x}, \hat{p})$ description and the $(\hat{a}_+, \hat{a}_-)$ description? Your answer should be a resounding "Yes!!" here.

    (c) $[\hat{x}, \hat{p}]$, $[\hat{a}_-, \hat{a}_+]$? $\hat{a}_-\psi_n, \hat{a}_+\psi_n$? $i\hbar$, 1, $\sqrt{n}\psi_{n-1}, \sqrt{n+1}\psi_n$ [L5 pages 2,3, L5 page 6, ...]

    (d) Parity of stationary states? e-o-e-o-... from the ground state. [L5 page 8, ...]

    (e) Can you quickly evaluate such things as $\langle \hat{x} \rangle$, $\langle \hat{V} \rangle$, $\langle \hat{p}^2 \rangle$ at *all* times for $\Psi(x,t)$, when an initial state $\Psi(x,0)$ is given as a mixture of a few stationary states? Always express $\hat{x}$ and $\hat{p}$ in terms of $\hat{a}_+$ and $\hat{a}_-$ and then use the last two answers of (c). Use orthonormality (and parity) to reduce integrals quickly. [HW 4.2 (prob 2.13), HW 4.3 (prob 2.41), Example 2.4,5, prob 2.11,15, ...]

12. Free particle [L6!]

    (a) What is the matter with this problem? What are the symptoms? [Too much freedom. No such thing.] Non-normalizable $\psi_k(x)$!

    (b) What are the ways out, which we use in this course, to deal with this problem? (1) Accept $\psi_k(x)$ as a stationary state, but not as a physical state. Or (2) accept it as a physical state, but only as a scattering state. [There is the third solution -- accept it as a physical state, but in a finite volume. This solution is, by strategy, not adopted in this course, but is genearlly well accepted in other courses. So just be aware.]

    (c) What is the Dirac delta function, and what does it have to with free particle stationary states? $\delta(x) = 0$ if x is non-zero and $\int dx \delta(x) = 1$, defines the Dirac delta function. For free particle stationary state $\psi_k(x) \sim \exp(ikx)$ it is important since $\int dx \exp(ikx) = 2\pi\delta(k)$, giving the nice properties mentioned above in I.b.ii [L4 page 4, L6 page 3, ...]

    (d) What is the nature of the stationary state $\psi_k(x)$, other than the fact that it is an energy eigenstate? It is a momentum eigenstate, $\hat{p}\psi_k = \hbar k \psi_k$.

13. Wave packet – Why is it essential? What is the rough way to characterize it? What is the meaning of the group velocity? What are the meanings of $\Psi(x,t)$ and $\phi(k)$, in relation to the Heisenberg Heisenberg Uncertainty Principle? It provides a way to form a normalizable wave function based on un-normalizable plane wave stationary states of the free particle problem. It can be characterized by the position and the width, in position space $\Psi(x,t)$ and also in momentum space $\phi(k)$. The Heisenberg principle is simply the fact that if you make $\Psi(x,t)$ narrow then you make $\phi(k)$ wide, and conversely. [L6 pages 3,5,6, ...]

14. Symmetry Principles [L4 pages 1,2,3, HW 3.3 (prob 2.36), ...]

    (a) What is the consequence on $\psi(x)$ if $V(x) = V(-x)$? $\psi(x)$ and $\psi(-x)$ are both solutions, if different. $\psi(x)$ *can* be taken as even or odd, although we don't have to.

    (b) What is the consequence on $\psi(x)$ if $V(x)^* = V(x)$? $\psi(x)$ and $\psi(x)^*$ are both solutions, if different. $\psi(x)$ *can* be taken as real, although we don't have to.

    (c) When/why is the E real? When the potential is real.

15. Conservation Principles

    (a) What is the QM statement for the energy conservation? Does that hold for all cases that we studied so far? Can you explain using the general solution for SE? $\frac{d}{dt}\langle \hat{H} \rangle = 0$ for *any* $\Psi(x,t)$. Yes. $\langle \hat{H} \rangle = \int dx \Psi(x,t)^* \hat{H} \Psi(x,t)$. Expand $\Psi(x,t)$ in terms of stationary states. Note that $\hat{H}$ applied to each stationary state is just a number (E_n or E_k) times the stationary state. Use the ortho-normality to see that there is no time dependence left in $\langle \hat{H} \rangle$. [L4 page 10, ...]

(b) In the free particle problem, the momentum should be conserved. What is the QM statement for that? Can you explain how it comes about? `$\frac{d}{dt}\langle\hat{p}\rangle = 0$ for` *`any`* `$\Psi(x,t)$. $\langle\hat{p}\rangle = \int dx \Psi(x,t)^* \hat{p} \Psi(x,t)$. Expand $\Psi(x,t)$ in terms of stationary states, which are in this case` *`momentum`* `eigenstates as well as energy eigenstates. Then, proceed like in (a), to show that there is no time dependence left in $\langle\hat{p}\rangle$. [L6 page 4, ...]`

(c) Consider a symmetric potential $V(x)$ with respect to certain x value, like 0 or $a/2$. If you form an even parity or an odd parity solution, does it stay that way? `Yes. If $\psi(x)$ has an even or odd parity, so does $\exp(-iEt/\hbar)\psi(x)$. So, if one starts with a linear combination of $\psi(x)$'s of the` *`same`* `parity, then the parity cannot change due to time evolution. [HW 3.4 (prob 2.37), Quiz 4.2, ...]`

16. By looking at a potential and energy, can you figure out whether you are in the "quantized/bound state" regime or in the "continuum/scattering state" regime? `$E < V(\infty)$` *`and`* `$E < V(-\infty)$? Then, quantized. Otherwise, continuum. [L7 page 1, ...]`

17. By looking at a potential and energy, can you qualitatively figure out what the wave function should look like (wavy, or exponential, boundary conditions of the wave function, where the amplitude is greatest and so on). `Always, see where the energy lies. If enery is less than the potential -- exponential decay behavior in general. If energy is greater than the potential -- wavy behavior in general. Note that wave functions should connect smoothly as long as the potential is finite, since both ψ and ψ' are continuous then. [L7 page 10, ...]`

18. Important in general, but happens to be only marginally important for midterm: Classical limit. Ehernfest theorem. Scattering problem (*non-symmetric* solution), tunneling, resonance, bound states and parity, etc...