For Test 2, some questions will be selected at random from the list below. Answers should in general be brief, but contain sufficient information to judge that you know the answer. Example: "What is the Fermi energy?" You cannot answer just "E_F" in a terse manner, but you need to explain physically that it is the energy of the electron with the highest energy in the many electron ground state, or related variations.

(1) Describe qualitatively the "free electron gas" approximation for solids.

(2) What is the definition of the Fermi energy of electrons in a crystal? Is the Fermi energy comparable, much larger, or much smaller than the total energy in a metal within the free electron gas approximation?

(3) What is the relation between the Fermi energy and the electronic density within the free electron gas approximation?

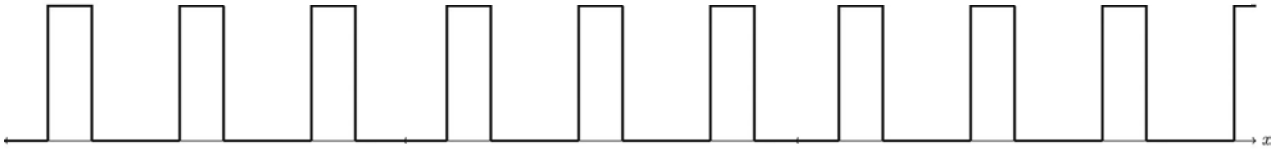
(4) What is the typical value of the Fermi temperature in Kelvin degrees? How it compares with room temperature? Is it a reasonable approximation to say that electrons in metals are always "cold" at room temperature?

(5) If you represent a crystal by a periodic potential V(x) with period "a", such that V(x+a) = V(x), what does the Bloch's theorem say? Write the formula linking $\psi(x+a)$ and $\psi(x)$. What is the relation between the probabilities $|\psi(x+a)|^2$ and $|\psi(x)|^2$?

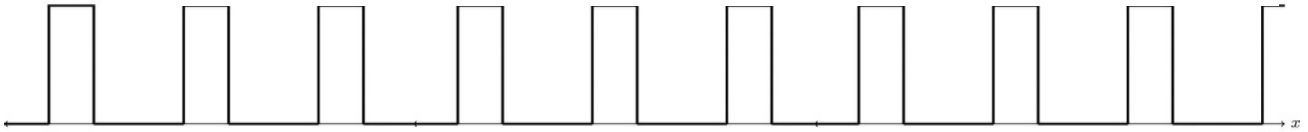
(6) Of the two approximations we learned to describe electrons in solids, the free electron gas and the periodic potential, which one predicts the existence of insulators? Explain verbally what an energy gap in an insulator is.

(7) Within the Dirac comb potential, for what values of *d*, the number of conduction electrons per atom, the system is a metal? I.e. d even or odd? Explain with a sketch.

(8) For the potential shown in the figure, consider the ground state of each well. Make a crude drawing by hand of the wave function for Bloch momentum Q=0.



(9) Same as (8) but for $Q=\pi/a$



(10) Find in book or lectures the formula E_n^2 for second order perturbation theory of non-degenerate levels. Consider the infinite square well in 1D. In class, I showed you that if the perturbation H' is simply to shift uniformly the bottom by V_0 , the first order perturbation correction already gives the expected uniform shift of all levels by V_0 and I said "the rest of the corrections cancel". Looking at the formula of E_n^2, in particular at the numerator, can you prove that the second order correction cancels based on orthonormality of eigenstates? Explain.

(11) Consider the formula derived in class for the energy level split of a state with degeneracy 2 (say levels *a* and *b*) after they split due to a perturbation to first order. What is the condition on the matrix elements W_{ab} W_{ba} W_{aa} W_{bb} for the split of these two levels to be symmetric? (i.e. with one level going up by $+\Delta E$, while the other level going down by $-\Delta E$).

(12) Assuming the electron rest mass is $mc^2 = 0.511$ MeV, with $M=10^6$, and that the energy levels of the H atom are $E_n = -13.6\ eV/n^2$ find the value in eV of the relativistic correction of the H atom for n=2 and l=0. Use directly the formula derived in class or book, and a calculator.

(13) Explain intuitively what causes the spin-orbit coupling correction.

(14) Using the numbers provided in question (12), find the spin-orbit (SO) coupling correction in the H atom corresponding to level n=1 and l=0 i.e. the ground state. Use directly the formula for the SO correction in lectures or book. Reminder: j is fixed in this case because l=0 and s=1/2.

(15) Within the free electron gas approximation, we deduced that electrons, even at zero temperature, exert pressure over the walls of their container. Explain briefly why that happens qualitatively. Hint: Are electrons at rest at zero temperature or they continue oscillating in their ground states?

(16) Consider the 1D harmonic oscillator and its ground state n=0, which you may recall is "even" under $x \rightarrow -x$. Now consider a perturbation H' that is "odd" under $x \rightarrow -x$ such as sin(x). Without doing any integral explicitly, can you say whether E_0^1 will be zero or nonzero?

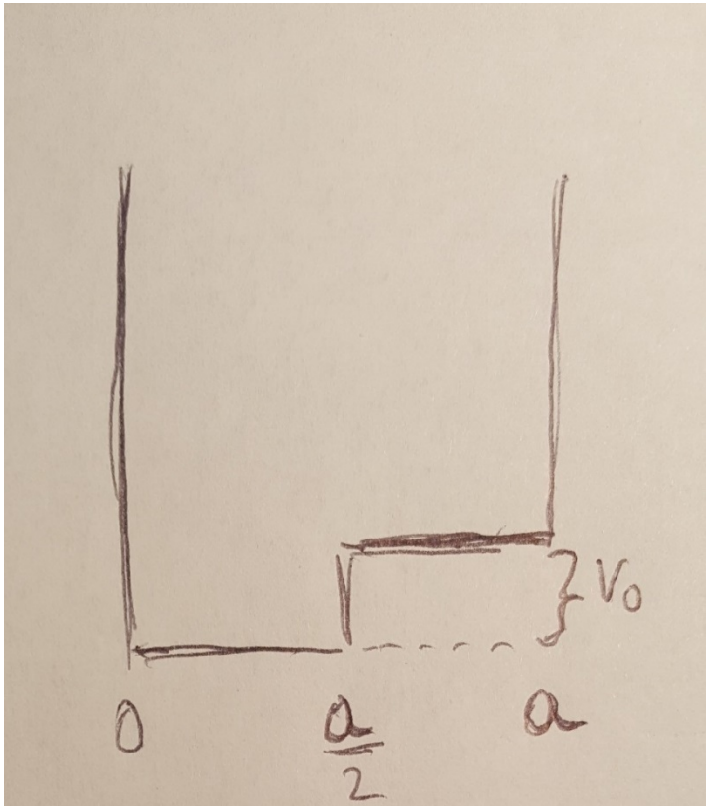
(17) Consider the entire fine structure correction shown in the last lecture. The final formula for the energy correction depends only on *n* and *j*. Consider the 5 “d” levels (i.e. l=2) corresponding to n=3 in the H atom. Including spin, how many total states we have before “turning on” the fine structure correction? How many total states we have after “turning on” the fine structure correction? Comment on the result.

(18) About question (17), namely still with n=3 l=2, after turning on the fine structure correction, how many multiples do I obtain i.e. how many values of j? How many states in each multiplet?

(19) Why in an atom with for example 68 electrons sometimes we say only *d*=3 contribute to the conduction and band formation? I.e. what happens to all the rest? Explain qualitatively.

(20) What are the periodic boundary conditions? Why they are mathematically useful?

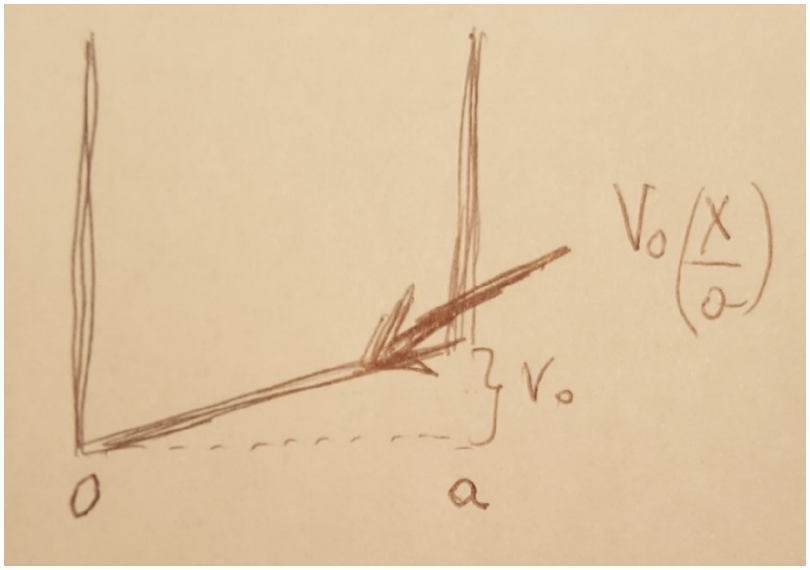
Example of first order perturbation theory



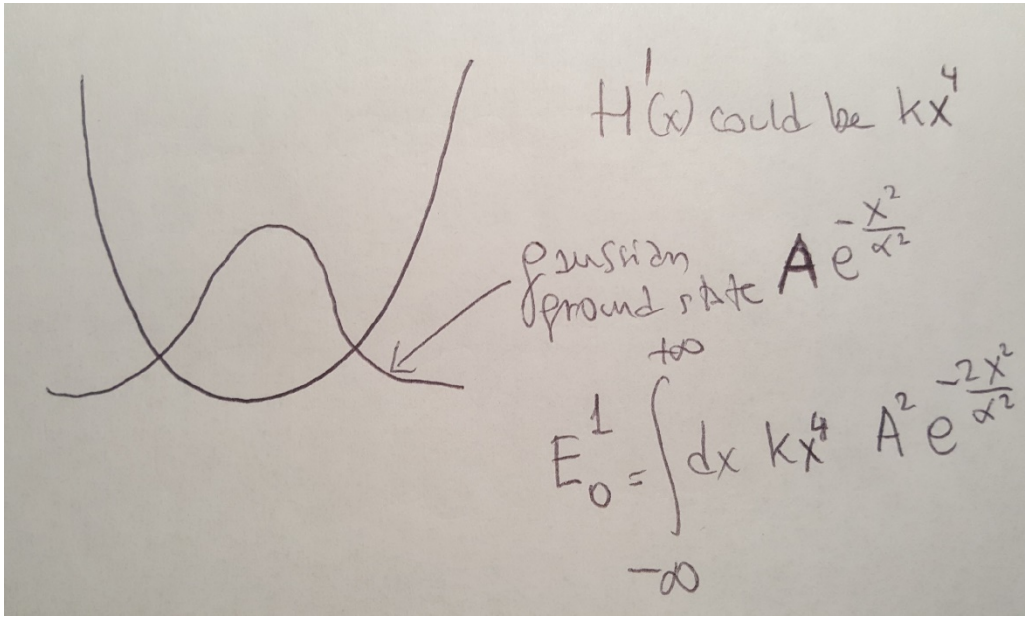
$$E_1^1 = \int_{\frac{a}{2}}^{a} dx \; V_0 \left[\sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) \right]^2$$

$$E_2^1 = \int_{a/2}^{a} dx \; V_0 \left[\sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right) \right]^2$$

Other examples of first order perturbation theory

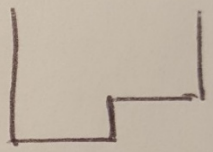


$$E_1^1 = \int_0^a dx \; V_0\left(\frac{x}{a}\right)\left[\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)\right]^2$$



Example of second order perturbation theory

∞ square well 1D again
Consider ground state $n = 1$.
Consider the same profile
as in previous page →



but go to second order keeping only
the first 2 terms in the sum.

$$E_1^{(2)} = \sum_{m \neq 1} \frac{|\langle \psi_m^{(0)} | H' | \psi_1^{(0)} \rangle|^2}{E_1^{(0)} - E_m^{(0)}} \approx \frac{|\langle \psi_2^{(0)} | H' | \psi_1^{(0)} \rangle|^2}{E_1^{(0)} - E_2^{(0)}} + \frac{|\langle \psi_3^{(0)} | H' | \psi_1^{(0)} \rangle|^2}{E_1^{(0)} - E_3^{(0)}}$$

in general

$$\psi_1^{(0)} = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right), \quad \psi_2^{(0)} = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right), \quad \psi_3 = \sqrt{\frac{2}{a}} \sin\left(\frac{3\pi x}{a}\right)$$

$$E_n^{(0)} = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

$$\langle \psi_2^{(0)} | H' | \psi_1^{(0)} \rangle = \int_{a/2}^{a} dx \; V_0 \underbrace{\sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right)}_{\psi_2^{(0)*}} \underbrace{\sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right)}_{\psi_1^{(0)}}$$