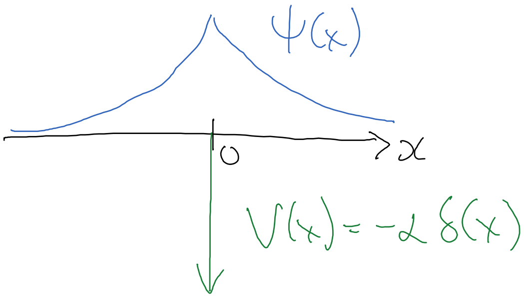
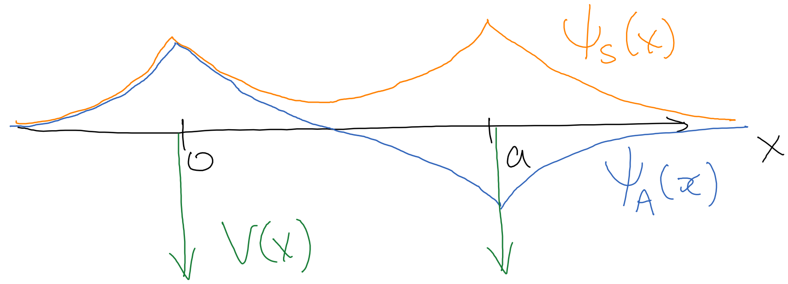
L61-Periodic Potential

Wednesday, February 17, 2016 07:34

* recall wave function of Dirac potential





for 2 nuclei, the wave functions look like combinations of the single-δ wave functions (symmetric/antisymmetric)

- as $a \to \infty$ the two energies become nearly degenerate.
- N nuclei support N symmetric/antisymmetric states
- As $N \to \infty$ these ∞ states form a continuous band.

* Bloch's theorem: if $V(x+a) = V(a)$ with periodic boundary conditions, then $H\psi = E\psi$ has periodic eigenfunctions $\psi(x+a) = e^{iKa}\psi(x)$ where K depends on E, not x.

- note: $\psi(x+a) \neq \psi(x)$ but $|\psi(x+a)|^2 = |\psi(x)|$ as expected
  this is similar to spin, where $R_{360}\chi = -\chi$ but $|\chi|^2$ is invariant

proof: let $D[\psi(x)] = \psi(x+a)$ translation operator.
since $\mathcal{H}$ is periodic, $[\mathcal{H}, D] = 0$.

ie. $\mathcal{H}D\psi(x) = \mathcal{H}(x)\psi(x+a) = \mathcal{H}(x+a)\psi(x+a) = D[\mathcal{H}(x)\psi(x)] = D\mathcal{H}\psi(x)$

Thus, there are simultaneous eigenfunctions of $\mathcal{H}$ and D

$\psi(x+a) = D\psi(x) = \lambda\psi(x) = e^{iKa}\psi(x)$ $\qquad \lambda = e^{iKa}$

Period B.C.'s: $\psi(x+Na) = e^{iKNa}\psi(x) \Rightarrow \left(e^{iKa}\right)^N = 1$

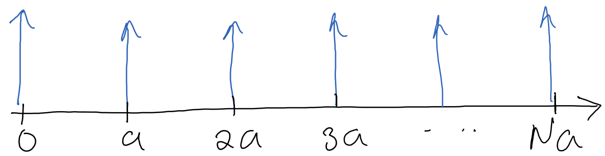
the N N^{th} roots of unity are: $Ka = 2\pi \frac{n}{N} \quad n = 0, 1, \ldots N-1$

Thus, periodic potentials have "phase-offset periodic" solutions.

* Band structure: an important feature of periodic potentials

consider the "Dirac comb" potential: $V(x) = \sum_{j=0}^{N-1} \alpha\, \delta(x - ja)$

with B.C.'s: $\psi(Na) = \psi(0)$
$\psi'(Na) = \psi'(0)$



this is a free particle between δ's.

$\psi_+(x) = A\sin(kx) + B\cos(kx)$ on $0 < x < a$ where $E = \frac{\hbar^2 k^2}{2m}$

$\psi_-(x) = e^{-iKa}\left[A\sin(k(x+a)) + B\cos(k(x+a))\right]$ $-a < x < 0$ (Bloch's theorem)

B.C.'s: $\psi_+(0) - \psi_-(0) = 0 \qquad B - e^{-iKa}(A\sin ka + B\cos ka) = 0 \qquad$ (I)

$\psi_+'(0) - \psi_-'(0) = \frac{2m\alpha}{\hbar^2}\psi(0) \qquad kA - e^{-iKa}\cdot k(A\cos ka - B\sin ka) = \frac{2m\alpha}{\hbar^2} B \qquad$ (II)

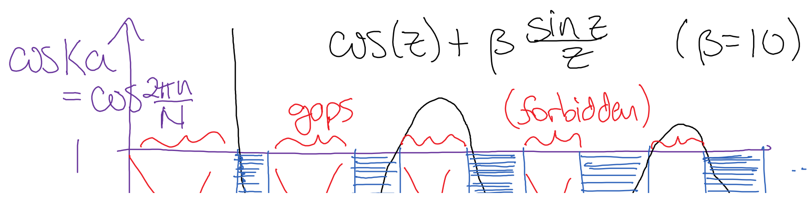
I: $A\sin ka = \left(e^{iKa} - \cos ka\right)B$, substitute A into (II) $\times \frac{\sin ka}{Bk}$:

$$\left(e^{iKa} - \cos ka\right)\left(1 - e^{-iKa}\cos ka\right) + e^{-iKa}\sin^2 ka = \frac{2m\alpha}{\hbar^2 k}\sin ka$$

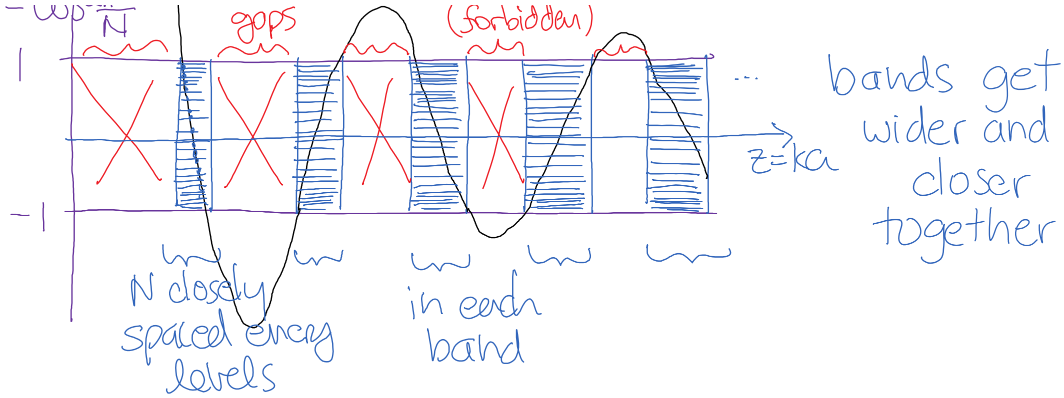
$$e^{iKa} - 2\cos ka + e^{-iKa}\left(\overbrace{\cos^2 ka + \sin^2 ka}^{=1}\right) = 2\frac{m\alpha}{\hbar^2 k}\sin ka$$

$$\cos Ka = \cos \underbrace{ka}_{z} + \underbrace{\frac{ma\alpha}{\hbar^2}}_{\beta}\frac{\sin ka}{ka} = \cos z + \beta\,\mathrm{sinc}\, z = f(z)$$

recall that $Ka = 2\pi\frac{n}{N}$ almost continuous $0 \le Ka < 2\pi$



. . . bands get



* fermions fill 2 e^- per single-particle state.
  let there be q free electrons / atom

then insulator for $q = 0, 2, 4, \ldots$ Cu : $\rho = 1.7\,\mu\Omega\cdot\text{cm}$ $(\times 10^{-6})$
conductor for $q \neq 0, 2, 4, \ldots$ Quartz: $\rho = 75\,\text{E}\Omega\cdot\text{cm}$ $(\times 10^{18})$
semiconductor for $q \approx 0, 2, 4$ close to the edges 25 orders of magnitude!