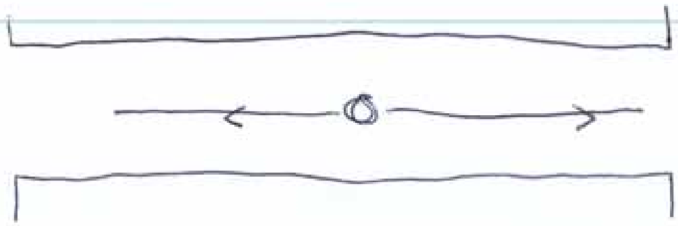
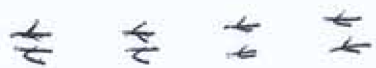
13.12 A

In each case, the "root" state is what you get by injecting a charge in the middle

no flux



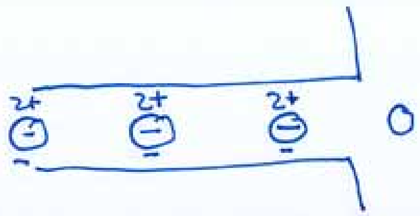
staggered flux



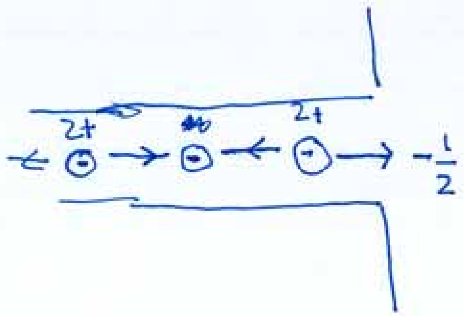
13.3 Divalent ions

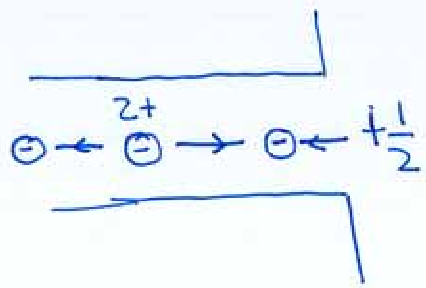
13.3.1 New phenomena arise for divalent ions, e.g. a $CaCl_2$ solution.

Consider an array of embedded $\ominus$ charges. We have again a "full" ground state

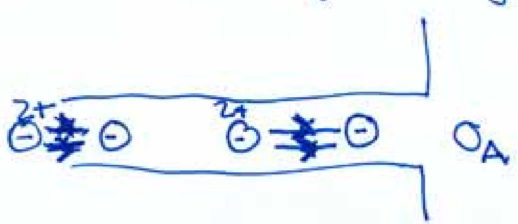


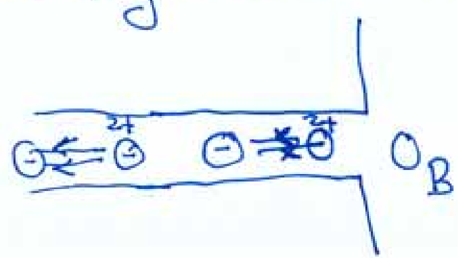
but now there are two quasi-degenerate empty (neutral) ground states

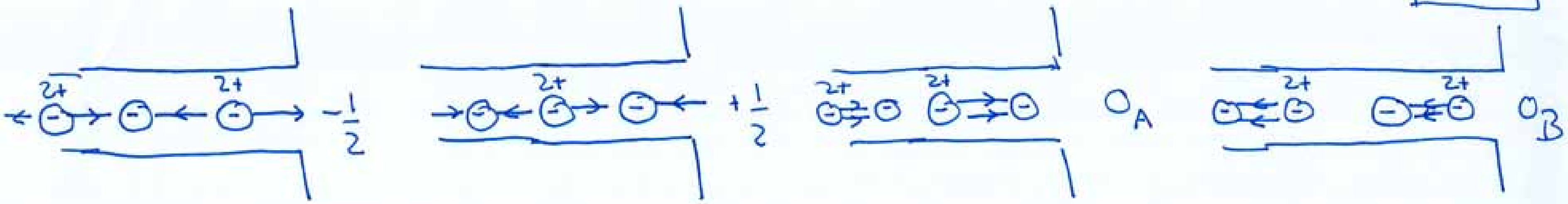




and two quasi-degenerate empty critical states







The transport cycle (~~positive~~ negative charge down the channel) looks to be

$$
\begin{array}{l}
-\frac{1}{2} \longrightarrow O_B \\
\qquad \Big\downarrow \text{snap} \\
\qquad O_A \longrightarrow +\frac{1}{2}
\end{array}
$$

At O_B, there is no energetic cost for adding

It transports <u>one</u> unit of charge.

Similarly for positive charge it is

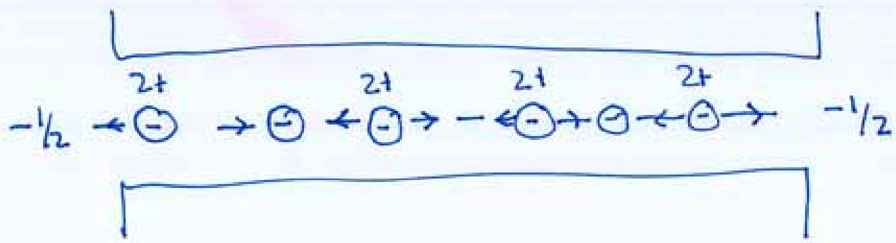
$$
\begin{array}{l}
+\frac{1}{2} \longrightarrow O_A \\
\qquad \Big\downarrow \text{snap} \\
\qquad O_B \longrightarrow -\frac{1}{2}
\end{array}
$$

— even though the transport is by charge 2 ions.

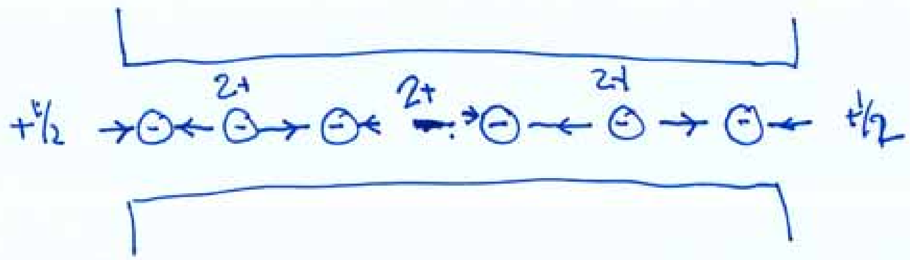
The central point is, that it's never necessary to let the flux build beyond $\mp$: You have $\ominus$ or $\overset{2+}{\ominus}$ available to flip it modulo 2!

This whole story is remarkably similar to the polyacetylene story.

Also: A Cl^- ion inside induces a soliton!



charge 1



charge -1

It's not inconceivable that one could set up nanoelectronic 'wires' with similar effects in the quantum regime.

· Minimax transport $\rightarrow$ tunneling

free energy barrier $\rightarrow$ instanton action

13.4 Some formal theory

13.4.1 We want the partition function for N positive and N' negative charges in the 1d interval $[-L/2, L/2]$. We also allow for boundary charges q, q'.

$$U = \frac{1}{2} \sum_{i,j=1}^{N+N'} \sigma_i \sigma_j \Phi(x_i - x_j) \qquad \sigma_\ell = \pm \text{ appropriately}$$

$$\Phi(x) = \underset{\uparrow \text{self-energy}}{\Phi(0)} - eE_0 |x|$$

$$U(q,q') = \frac{1}{2} \int dx\, dx' \, \rho(x) \Phi(x-x') \rho(x')$$

$$\rho(x) = \sum_{j=1}^{N+N'} \sigma_j \delta(x - x_j) + q\delta(x + L/2) + q' \delta(x - L/2)$$

$$Z(q,q') = \sum_{N,N'=0}^{\infty} e^{\mu(N+N')/T} \frac{1}{N!\,N'!} \left\{ \prod_{j=1}^{N+N'} \frac{\pi a^2}{\ell_0^2} \int_{-L/2}^{L/2} \frac{dx_j}{\ell_0} \right\} e^{-U(q,q')/T}$$

$$c = e^{\mu/T}/\ell_0^3 \quad (\text{same for both } \pm 1)$$

Insert

$$1 = \int \mathcal{D}\rho(x)\, \delta\big(\rho(x) - \underset{\substack{\uparrow \\ \text{from previous} \\ \text{page}\ldots}}{\Sigma \cdots}\big) = \iint \mathcal{D}\rho(x)\, \mathcal{D}\theta(x)\, \exp\left\{-i \int_{-L/2}^{L/2} \theta(x) \left(\rho(x) - \Sigma\cdots\right)\right\}$$

functional integral

The exponent in Z is quadratic in ρ (through U.). We can perform the Gaussian integral by completing the square, and also do the sums on N and N'

$$Z(q,q') = \iint_{-\infty}^{\infty} \frac{d\theta_i}{2\pi} \frac{d\theta_f}{2\pi}\, e^{i(q\theta_i + q'\theta_f)} \iint \mathcal{D}\rho\, \mathcal{D}\theta\, \tilde{S}$$

$(\theta_i \equiv \theta(-L/2)\,,\ \theta_f \equiv \theta(+L/2))$

$$\tilde{S} \equiv \sum_{N=0}^{\infty} \frac{1}{N!} e^{\mu N/T} \left(\frac{\pi a^2}{\ell_0^3} \int dx\, e^{i\theta(x)}\right)^N \sum_{N'=0}^{\infty} \frac{1}{N'!} e^{\mu N/T} \left[\frac{\pi a^2}{\ell_0^3} \int dx\, e^{-i\theta(x)}\right] \times$$

$$\times\, e^{-\frac{1}{2} \iint_{-L/2}^{L/2} dx\, dx'\, \rho(x)\, \Phi(x-x')\, \rho(x') - i \int_{-L/2}^{L/2} dx\, \theta(x)\, \rho(x)}$$

$\boxed{\cancel{H\rho\, 2 e^{-1}}\ \cancel{\Sigma} \int \cancel{\mathcal{D}}\rho(x)\, \cancel{e^{\frac{1}{2}\rho(x)\Phi\rho(x)}} +}$

$$\Gamma \int \mathcal{D}\rho \, e^{-\frac{1}{2}\rho M \rho + A\rho} \rightarrow \int \mathcal{D}\rho \, e^{-\frac{1}{2}(\rho - AM^{-1}) M (\rho - M^{-1}A)} e^{+\frac{1}{2} AM^{-1}A}$$

$$\rightarrow \# \, e^{\frac{1}{2} AM^{-1}A} \quad \lrcorner$$

$$Z(q,q') = \iint_{-\infty}^{\infty} \frac{d\theta_i}{2\pi} \frac{d\theta_f}{2\pi} \int \mathcal{D}\theta \, e^{-S}$$

$$S = \frac{T}{2} \iint_{-L/2}^{L/2} dx\, dx' \, \theta(x) \, \Phi^{-1}(x-x') \, \theta(x') - 2\pi a^2 c \int_{-L/2}^{L/2} dx \cos\theta(x)$$

operator inverse

But $\Phi^{-1}(x-x') = -(2eE_0)^{-1} \delta(x-x') \partial_{x'}^2$

$$\Gamma \int dx' \, \delta(x-x') \underbrace{\partial_{x'}^2 |x'-x''|}_{\hookrightarrow \partial_{x'} \sqcup \;\hookrightarrow \delta(x'-x'')} \doteq \delta(x-x'') \quad \lrcorner$$

so
$$e^{-S} = \int \mathcal{D}\theta(x)\, e^{-\frac{x_T}{2}\int dx \left\{ \frac{1}{2}(\partial_x\theta)^2 - \frac{4\alpha}{x_T^2}\cos\theta \right\}}$$

subject to $\theta(-L/2) = \theta_i \quad \theta(L/2) = \theta_f$

This is the expression we'd get for the amplitude ~~of~~ for a transition from θ_i to θ_f in imaginary time (in quantum theory!). We can throw the whole apparatus of band theory (spectral analysis), etc. at it.

x_T and α emerge again as the characteristic parameters.