Atomic Limit

$$H_0 = \epsilon_d (n_{d\uparrow} + n_{d\downarrow}) + U n_\uparrow n_\downarrow$$

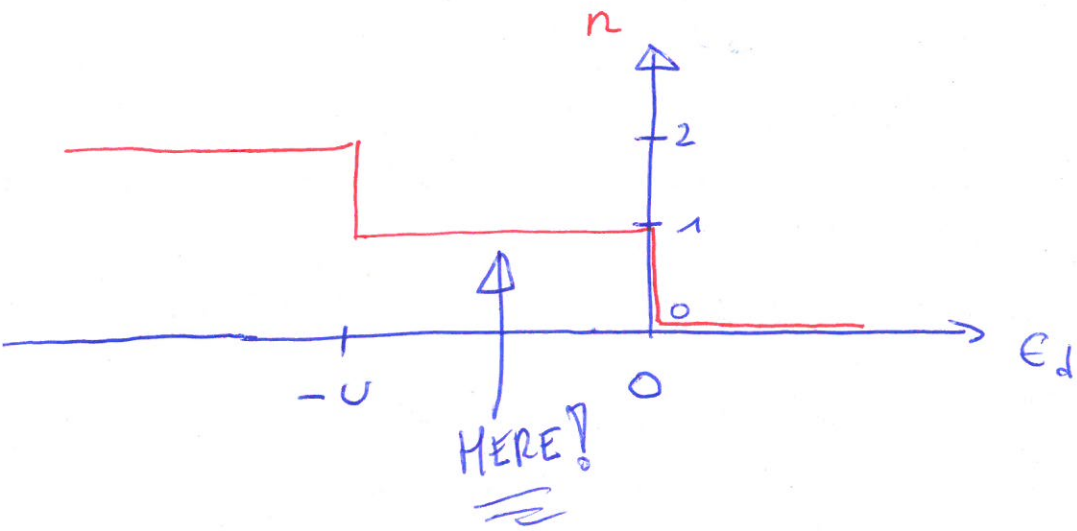
Four electronic states:

$|0\rangle \to E_0 = 0$ charge $n = n_\uparrow + n_\downarrow = 0$

$|\uparrow\rangle \to E_\uparrow = \epsilon_d$ charge $n = 1$

$|\downarrow\rangle \to E_\downarrow = \epsilon_d$ charge $n = 1$

$|\uparrow\downarrow\rangle \to E_{\uparrow\downarrow} = 2\epsilon_d + U$ charge $n = 2$



$U > 0$

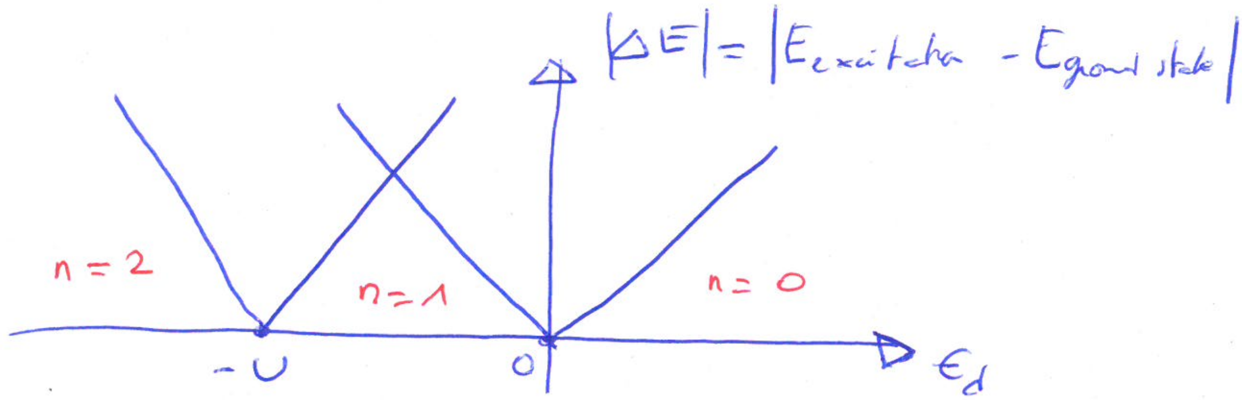
$k_B T = 0$

For $\epsilon_d = -\frac{U}{2}$, charge is well frozen in the $n=1$ state

$\Rightarrow$ local moment $|\uparrow\rangle$ or $|\downarrow\rangle$

<u>Note</u>: this is different from the working point of the Cooper pair box qubit, where one tunes on the degeneracy $n=0$, $n=1$ (no spin!).

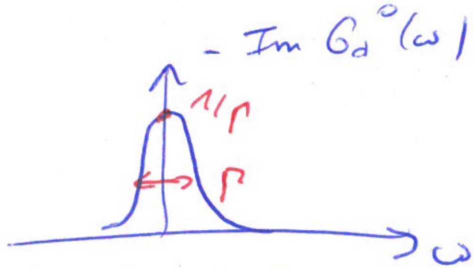
Transition from spin degenerate ground state



Perturbation at order U^2

- ## Resonant level $U=0$

$$G_d^0(\omega) = \frac{1}{\omega + i\Gamma}$$



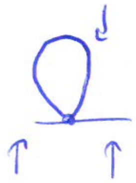
retarded Green's f^t $\langle d^\dagger(\omega) d(\omega)\rangle$

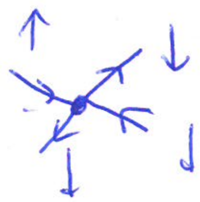
- ## Lowest order self energy

Take $\epsilon_d = -\frac{U}{2}$, so that

charge $\langle n_\uparrow + n_\downarrow \rangle = 1$ exactly $\forall U$

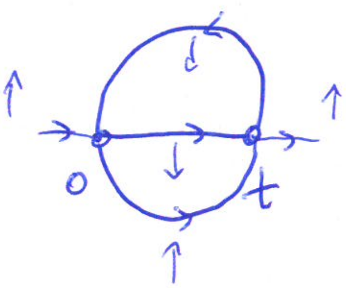
(prove it with particle-hole transformat°)

$\Rightarrow$  $= 0$

where we note the vertex  $= U$

from $U n_\uparrow n_\downarrow = U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow$

The lowest order diagram is

 $= \Sigma(t) = U^2 \left[G_d^0(t) \right]^3$

$$\Sigma(t) \propto U^2 \frac{i}{t^3} \quad \text{at} \quad t \gg \frac{1}{\Gamma}$$

since $G_d^0(t) \propto \frac{i}{t}$ at $t \gg \frac{1}{\Gamma}$

Note that $G_d^0(t)$ and $\Sigma(t)$ are <u>regular</u> for $t = 0$

$$\Rightarrow \Sigma(\omega) = \int_0^{+\infty} dt \, e^{i\omega t} \, \Sigma(t)$$

is regular also.

dimensionless number

$$\Rightarrow \underset{\omega \to 0}{\Sigma(\omega)} = -a \frac{U^2}{\Gamma^2} \omega + i b \frac{U^2}{\Gamma^3} \omega^2$$

$$\Sigma(\omega) = \left(1 - \frac{1}{Z}\right) \omega + i \frac{\omega^2}{\Omega} \quad \text{for } \omega \to 0$$

with $1 - \frac{1}{Z} = -a \frac{U^2}{\Gamma^2}$

$$\boxed{Z = \frac{1}{1 + a \frac{U^2}{\Gamma^2}}}$$

for $U \lesssim \pi\Gamma$ (U not too large)

quasiparticle weight.

Interacting Green's function:

Let's drop Im Σ for simplicity.

as $G_d^0 = \frac{1}{\omega + i\Gamma}$

$$G_d(\omega) = \frac{1}{\left[G_d^0(\omega)\right]^{-1} - \Sigma(\omega)}$$

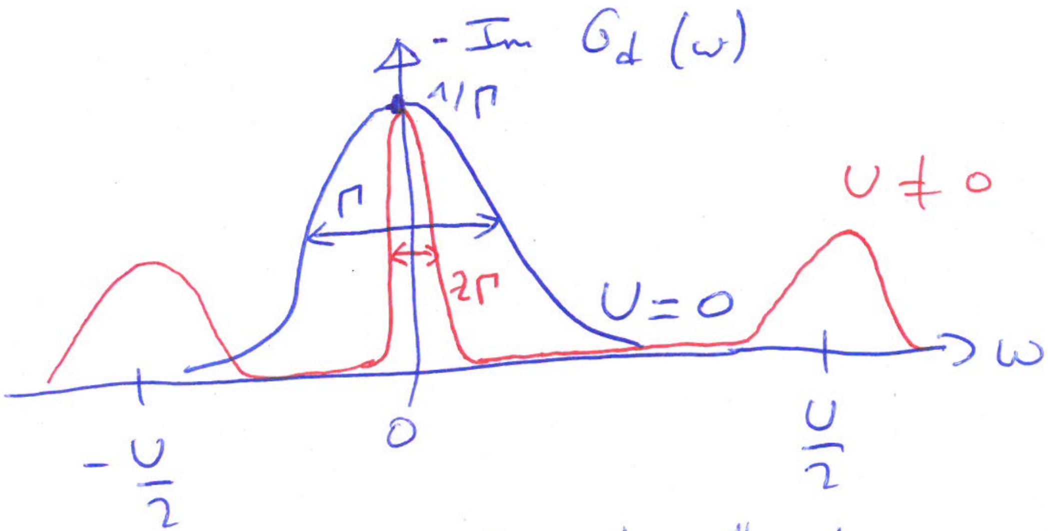
$$G_d(\omega) = \frac{1}{\omega + i\Gamma - \left(1 - \frac{1}{Z}\right)\omega}$$

$$G_d(\omega) = \frac{1}{\frac{\omega}{Z} + i\Gamma} = \frac{Z}{\omega + iZ\Gamma}$$

$\Rightarrow$ resonance of width $Z\Gamma < \Gamma$

and total weight $Z < 1$

$\left(Z \simeq \frac{1}{1 + a\frac{U^2}{\Gamma^2}} \quad \text{for} \quad U \lesssim \pi\Gamma \right)$



$G_d(\omega = 0) = \frac{1}{i\Gamma}$ is true to all orders in U (Friedel sum rule)

SCHRIEFFER – WOLFF TRANSFORMATION

- Goal:

derive an effective Hamiltonian in the subspace where the impurity has charge $n=1$ (spin doublet).

Total wavefunction $\Psi = \begin{pmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \end{pmatrix}$

has $|n=0\rangle$ has $|n=1\rangle$ has $|n=2\rangle$

OUR SUBSPACE

H = Anderson model

$$H\Psi = E\Psi$$

$$\Rightarrow \begin{pmatrix} H_{00} & H_{01} & 0 \\ H_{10} & H_{11} & H_{12} \\ 0 & H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \end{pmatrix} = E \begin{pmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \end{pmatrix}$$

no term like d^+d in H.

with $H_{nn'} = P_n H P_{n'}$

$P_0 = (1-n_\uparrow)(1-n_\downarrow)$ projector onto ψ_0

$P_1 = n_\uparrow + n_\downarrow - 2n_\uparrow n_\downarrow$ projector onto ψ_1

$\psi_2 = n_\uparrow n_\downarrow$ projector onto ψ_2

$$\left| \begin{aligned} &H_{00}\psi_0 + H_{01}\psi_1 = E\psi_0 \\ &H_{10}\psi_0 + H_{11}\psi_1 + H_{12}\psi_2 = E\psi_1 \\ &H_{21}\psi_1 + H_{22}\psi_2 = E\psi_2 \end{aligned} \right.$$

$$\Rightarrow \psi_0 = \frac{1}{E - H_{00}} H_{01}\psi_1$$

and $$\psi_2 = \frac{1}{E - H_{22}} H_{21}\psi_1$$

$$\Rightarrow \boxed{\left[H_{11} + H_{10}\frac{1}{E-H_{00}}H_{01} + H_{12}\frac{1}{E-H_{22}}H_{21}\right]\psi_1 = E\psi_1}$$

<u>exact</u> Schrödinger equation in subspace $n=1$

Let's compute H_{10} first term:

$$H_{10} = P_1 \sum_{k\sigma}\left(t d^\dagger_\sigma c_{k\sigma} + \cancel{t c^\dagger_{k\sigma} d_\sigma}\right) P_0$$

kills on P_0

$$H_{10} = P_1 \sum_{k\sigma} t d^\dagger_\sigma c_{k\sigma} P_0$$

$$H_{10} = \sum_{k\sigma} t \underbrace{(n_\uparrow + n_\downarrow - 2n_\uparrow n_\downarrow)}_{} d^\dagger_\sigma (1-n_\uparrow)(1-n_\downarrow) c_{k\sigma}$$

1 as $d^\dagger_\sigma (1-n_\uparrow)(1-n_\downarrow)$ is in the $n=2$ sector.

We can check that:

$$d^\dagger_\sigma (1-n_\uparrow)(1-n_\downarrow) = d^\dagger_\sigma (1-n_{-\sigma})$$

$$\Rightarrow H_{10} = \sum_{k\sigma} t d^\dagger_\sigma (1-n_{-\sigma}) c_{k\sigma}$$

Proof:

SWT ③

$$d^\dagger_\sigma (1-n_\uparrow)(1-n_\downarrow) \; |0\rangle = d^\dagger_\sigma |0\rangle$$
$$= d^\dagger_\sigma (1-n_{-\sigma}) |0\rangle$$

$$d^\dagger_\sigma (1-n_\uparrow)(1-n_\downarrow) |\pm\sigma\rangle = 0$$
$$d^\dagger_\sigma (1-n_{-\sigma}) \; |\sigma\rangle = d^\dagger_\sigma |\sigma\rangle = d^\dagger_\sigma d^\dagger_\sigma |0\rangle = 0$$
$$d^\dagger_\sigma \underbrace{(1-n_{-\sigma})}_{\text{zero}} \; |-\sigma\rangle = 0$$

$$d^\dagger_\sigma (1-n_\uparrow)(1-n_\downarrow) = |\uparrow\downarrow\rangle = 0$$
$$d^\dagger_\sigma (1-n_{-\sigma}) \; |\uparrow\downarrow\rangle = 0 \qquad \text{ok!}$$

Similarly:

$$H_{12} = \sum_{k\sigma} t \, d^\dagger_\sigma \, n_{-\sigma} \, c_{k\sigma}$$

and $H_{01} = H_{10}^\dagger$, $H_{21} = H_{12}^\dagger$.

Proof:

$$H_{12} = t \sum_{k\sigma} (n_\uparrow + n_\downarrow - 2 n_\uparrow n_\downarrow) \big(\cancel{d^\dagger_\sigma c_{k\sigma}} + c^\dagger_{k\sigma} d_\sigma\big) \, n_\uparrow n_\downarrow$$

kills a $|\uparrow\downarrow\rangle$

$$H_{12} = t \sum_{k\sigma} c^\dagger_{k\sigma} \underbrace{(n_\uparrow + n_\downarrow - 2 n_\uparrow n_\downarrow)}_{1} \underbrace{d_\sigma \; n_\uparrow n_\downarrow}$$

in the $n=1$ sector

$$H_{12} = t \sum_{k\sigma} c^\dagger_{k\sigma} \, d_\sigma \, n_\uparrow n_\downarrow$$

$$H_{12} = t \sum_{k\sigma} c^\dagger_{k\sigma} \, d_\sigma \, n_{-\sigma}$$

We can now express the effective Hamiltonian.

Let's consider first:

$$H_{12}\frac{1}{E-H_{22}}H_{21} = t^2 \sum_{\substack{kk' \\ \sigma\sigma'}} \underbrace{c^+_{k\sigma} d_\sigma n_{-\sigma} \frac{1}{E-H_{22}} n_{-\sigma'} d^+_{\sigma'} c_{k'\sigma'}}_{T^{\sigma\sigma'}}$$

$$\langle\Uparrow| T^{\sigma\sigma'} |\Uparrow\rangle = c^+_{k\sigma} \underbrace{\langle\Uparrow| d_\sigma}_{\delta_{\sigma\downarrow}\langle\uparrow\downarrow|} n_{-\sigma} \frac{1}{E-H_{22}} n_{-\sigma'} \underbrace{d^+_{\sigma'}|\Uparrow\rangle}_{\delta_{\sigma'\downarrow}|\Uparrow\downarrow\rangle} c_{k\sigma'}$$

$$\ldots = \delta_{\sigma\downarrow}\delta_{\sigma'\downarrow}\, c^+_{k\downarrow} \langle\uparrow\downarrow| \hat{n}_\uparrow \frac{1}{E-H_{22}} \hat{n}_\uparrow |\uparrow\downarrow\rangle c_{k'\downarrow}$$

$$\ldots = \delta_{\sigma\downarrow}\delta_{\sigma'\downarrow}\, c^+_{k\downarrow} \frac{1}{E-H_{22}} c_{k'\downarrow}$$

But $E \simeq \epsilon_d$

and $H_{22} \simeq 2\epsilon_d + U - \epsilon_{k'}$

due to removal of electron.

$$\Rightarrow \langle\uparrow| T^{\sigma\sigma'} |\Uparrow\rangle \simeq \delta_{\sigma\downarrow}\delta_{\sigma'\downarrow} \frac{-t^2}{U+\epsilon_d-\epsilon_{k'}} c^+_{k\downarrow} c_{k'\downarrow}$$

Now for the spin flip term:

$$\langle\Uparrow| T^{\sigma\sigma'} |\Downarrow\rangle = \delta_{\sigma\Uparrow}\delta_{\sigma'\downarrow} \frac{-t^2}{U+\epsilon_d-\epsilon_{k'}} c^+_{k\Uparrow} c_{k'\downarrow}$$

Assume $U+\epsilon_d \gg |\epsilon_k|$

$$H_{12} \frac{1}{E-H_{22}} H_{21} = \sum_{\substack{kk' \\ \sigma\sigma'}} c^{+}_{k\sigma} c_{k'\sigma'} d^{+}_{\sigma'} d_{\sigma} \frac{t^2}{U+\epsilon_d}$$

forget projector in subspace

$$= \frac{t^2}{U+\epsilon_d} \sum_{kk'} \Big[c^{+}_{k\uparrow} c_{k'\downarrow} d^{+}_{\downarrow} d_{\uparrow} + h.c. +$$

$$+ c^{+}_{k\uparrow} c_{k'\uparrow} d^{+}_{\uparrow} d_{\uparrow} + c^{+}_{k\downarrow} c_{k\downarrow} d^{+}_{\downarrow} d_{\downarrow} \Big]$$

We introduce
$$\left| \begin{array}{l} \sigma^{+} = d^{+}_{\uparrow} d_{\downarrow} \\ \sigma^{-} = d^{+}_{\downarrow} d_{\uparrow} \\ \sigma^{z} = d^{+}_{\uparrow} d_{\uparrow} - d^{+}_{\downarrow} d_{\downarrow} \end{array} \right.$$

within the subspace. $n = d^{+}_{\uparrow} d_{\uparrow} + d^{+}_{\downarrow} d_{\downarrow} = 1$

$$\Rightarrow \left| \begin{array}{l} d^{+}_{\uparrow} d_{\uparrow} = \frac{d^{+}_{\uparrow} d_{\uparrow} - d^{+}_{\downarrow} d_{\downarrow}}{2} + \frac{d^{+}_{\uparrow} d_{\uparrow} + d^{+}_{\downarrow} d_{\downarrow}}{2} \\ d^{+}_{\uparrow} d_{\uparrow} = \sigma^{z} + \frac{1}{2} \\ d^{+}_{\downarrow} d_{\downarrow} = \frac{d^{+}_{\uparrow} d_{\uparrow} + d^{+}_{\downarrow} d_{\downarrow}}{2} - \frac{d^{+}_{\uparrow} d_{\uparrow} - d^{+}_{\downarrow} d_{\downarrow}}{2} \\ d^{+}_{\downarrow} d_{\downarrow} = \frac{1}{2} - \sigma_{z} \end{array} \right.$$

$$H_{12} \frac{1}{E-H_{22}} H_{21} = \frac{t^2}{U+\epsilon_d} \sum_{kk'} \Big[c^{+}_{k\uparrow} c_{k'\downarrow} \sigma^{-} + h.c.$$

$$+ \frac{c^{+}_{k\uparrow} c_{k'\uparrow} - c^{+}_{k\downarrow} c_{k'\downarrow}}{2} \sigma^{z} +$$

$$+ \frac{c^{+}_{k\uparrow} c_{k'\uparrow} + c^{+}_{k\downarrow} c_{k'\downarrow}}{2} \Big]$$

Similarly:

$$H_{10} \frac{1}{E - H_{11}} H_{01} = \frac{-t^2}{\epsilon_d} \sum_{kk'} \Big[c^\dagger_{k\uparrow} c_{k'\downarrow} \sigma^- + h.c.$$

$$+ \frac{c^\dagger_{k\uparrow} c_{k'\uparrow} - c^\dagger_{k\downarrow} c_{k'\downarrow}}{2} \sigma^z - \frac{c^\dagger_{k\uparrow} c_{k'\uparrow} + c^\dagger_{k\downarrow} c_{k'\downarrow}}{2} \Big]$$

Introducing Pauli matrices $\vec{\tau}$ and $\vec{S} = \frac{\vec{\sigma}}{2}$

$$H_{eff} = \sum_{\substack{kk' \\ \alpha\alpha'}} \underbrace{\left(\frac{2t^2}{U + \epsilon_d} - \frac{2t^2}{\epsilon_d} \right)}_{J} c^\dagger_{k\alpha} \frac{\vec{\tau}_{\alpha\alpha'}}{2} c_{k'\alpha'} \cdot \vec{S}$$

+ potential term

$$\boxed{J = 2t^2 \left(\frac{1}{U + \epsilon_d} - \frac{1}{\epsilon_d} \right)}$$

for $\epsilon_d = -\frac{U}{2}$ (middle of charge state)

$$J = \frac{8t^2}{U} > 0 \quad \text{antiferromagnetic}$$

<u>Note:</u> J increases for $\epsilon_d \simeq 0$ and $U + \epsilon_d \simeq 0$ $\Rightarrow$ enhanced charge fluctuations enhance J