FYS4480/9480 Lectures November 28 & 29

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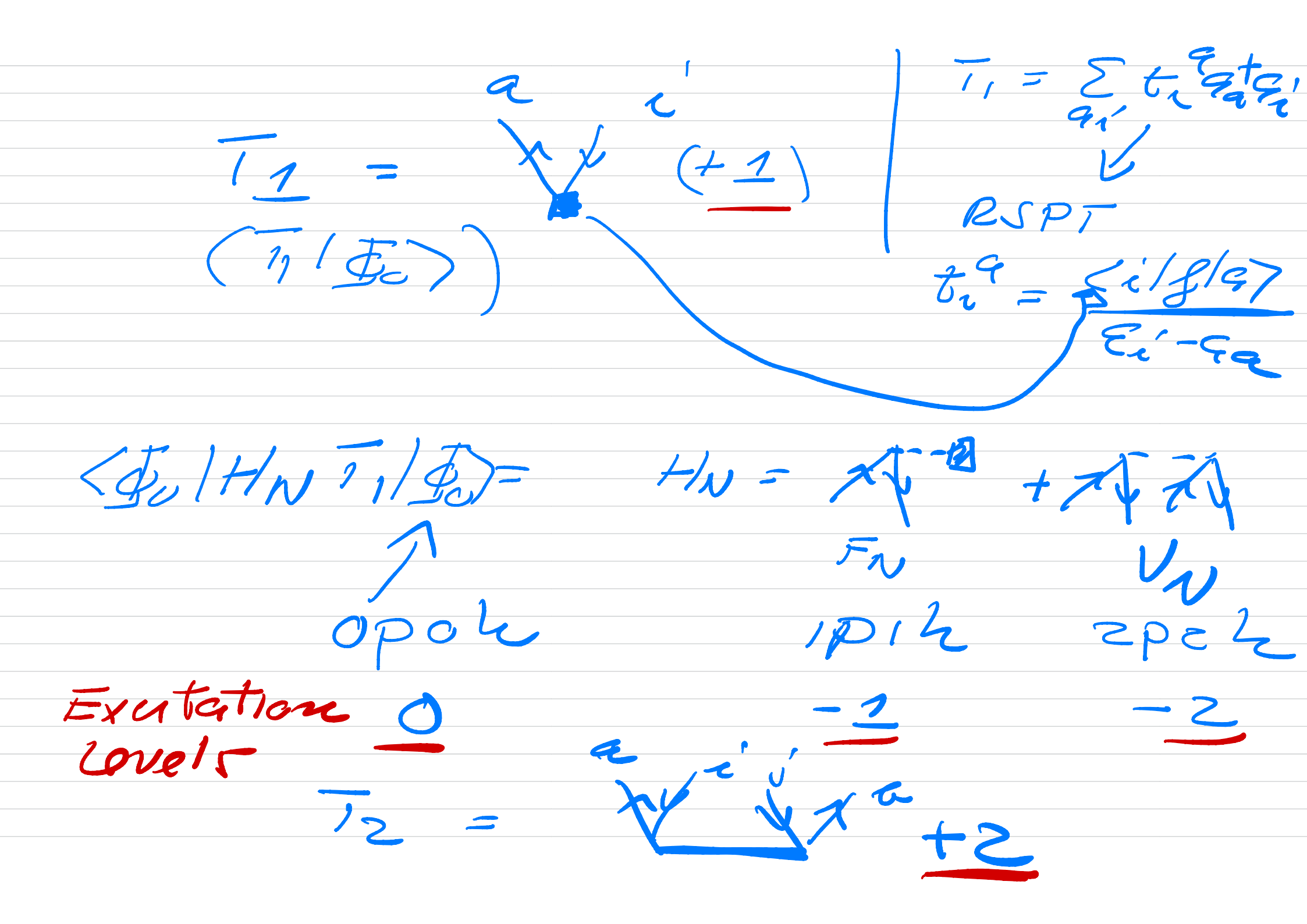
$$e^{-T} H_N e^{T} = H_N + [H_N, T] + \frac{1}{2}[[H_N, T], T] + \cdots$$

$H_N T$

$$\Delta E = \langle \Phi_0 | e^{-T} H_N e^{T} | \Phi_0 \rangle$$

$$\langle \Phi_i^a | e^{-T} H_N e^{T} | \Phi_0 \rangle = 0$$

$$\langle \Phi_{ij}^{ab} | e^{-T} H_N e^{T} | \Phi_0 \rangle = 0$$


$\bar{T}_1 = \sum_{q,i'} t_i^q a_q^\dagger a_{i'}$
RSPT
$t_i^q = \frac{\langle i'|f|q\rangle}{\varepsilon_{i'} - \varepsilon_q}$
$\bar{T}_1 = (\bar{T}_1|\Phi_0\rangle)$
a
i'
(+1)
$\langle\Phi_0|H_N\bar{T}_1|\Phi_0\rangle =$
opok
$H_N =$
F_N
+
V_N
1p1h
2p2h
Excitation levels
0
-1
-2
$\bar{T}_2 =$
a
i'
j'
a
+2

$$\frac{1}{4} \sum_{\substack{ab \\ ij}} \langle ab | v | ij \rangle t_{ij}^{ab}$$

$|ab\rangle \rightarrow A = \#$ configurations
$a\ b$

$|ij\rangle \rightarrow I$

$\langle ij | v | ab \rangle \rightarrow$

V_{IA}

$t_{ij}^{ab} \rightarrow t_{AI}$

$$\sum_{\substack{ab \\ ij}} \langle ab | v | ij \rangle t_{ij}^{ab} \rightarrow \sum_{IA} V_{IA} \cdot t_{AI}$$

$$= \hat{V} \cdot \hat{t}$$