IMPORTANCE OF ELECTRON-ELECTRON INTERACTION

EXAMPLE IONIZATION ENERGY OF NOBLE GASES

	Z	LAST OCCUPIED SHELL	IONIZATION ENERGY - INDEP. ELECTRON ($\frac{E_h}{n^2}$ (Ry))	EXP. - IONIZ. (Ry)
He	2	n=1	4	1.81
Ne	10	n=2	25	1.53
Ar	18	n=3	36	1.16
Kr	36	n=4	64	1.03
Xe	54	n=5	116,64	0.89

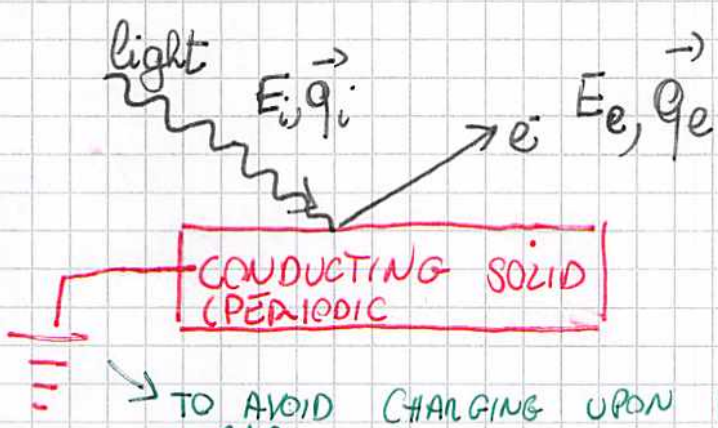
ELECTRONIC BANDS BASED ON BLOCH-THEOREM

VALID IN A SINGLE PARTICLE PICTURE

DO THE ELECTRONIC BAND EXISTS IN REALITY?

ANGLE RESOLVED PHOTOEMISSION SPECTROSCOPY (ARPES)

(IONISATION OF A SOLID)



→ TO AVOID CHARGING UPON MULTIPLE IONIZATION (AND COULOMB INTERACTION BETWEEN EXCAPING ELECTRON AND CHARGED SOLID)

ELECTRON - EXCAPS ONLY FROM FEW ATOMIC PLANE SURFACE OF THE SOLID PERIODIC $\{\vec{G}_{//}\}$ RECIPROCAL LATTICE OF THE SURFACE OR 2D MATERIAL (ONLY IN PLANE PERIODICITY)

- CONSERVATION OF ENERGY (GOOD QUANTUM NUMBER)

IN THE MATERIAL WE DEPOSIT AN ENERGY

$\therefore E = E_i - E_e$

GAS DISCHARGE

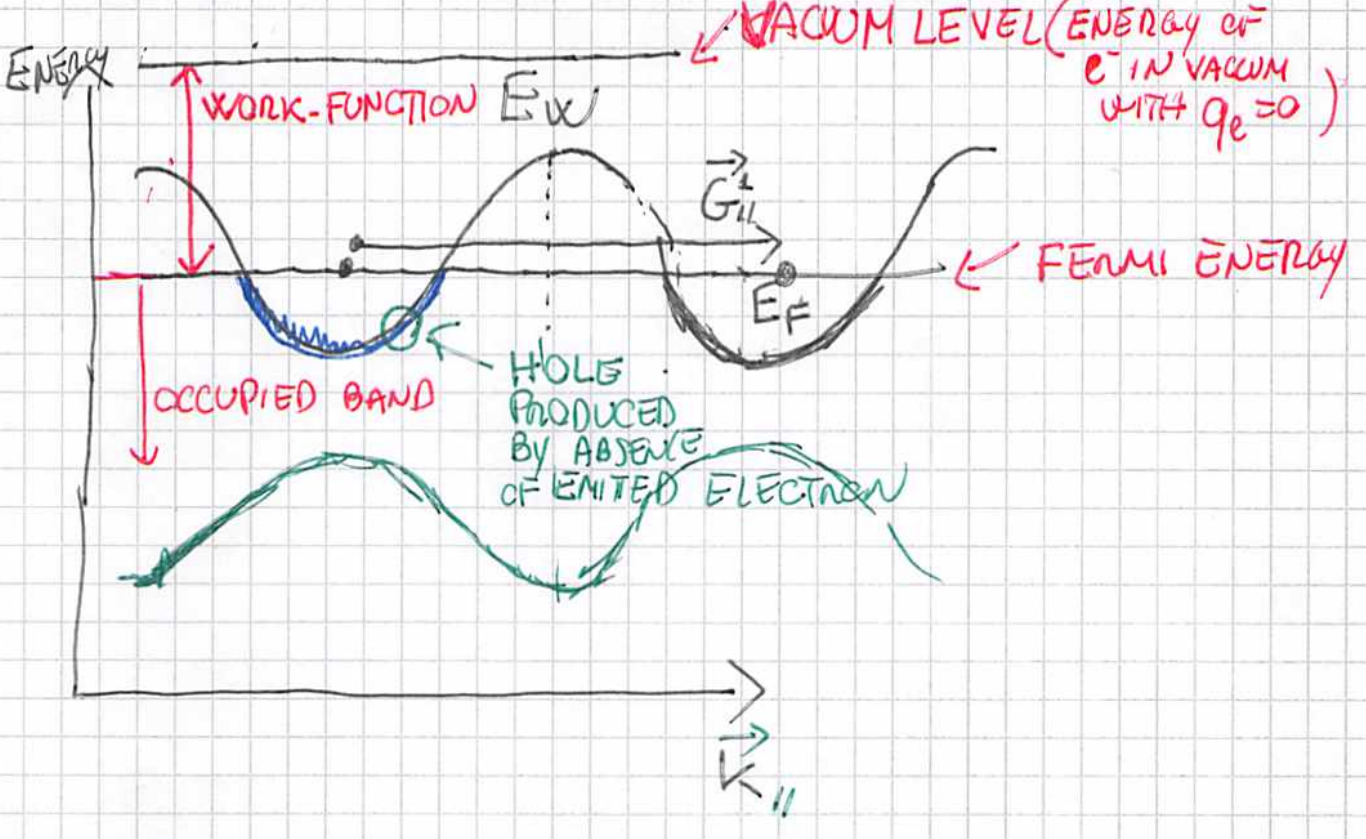
$E_i = 20\text{-}50$ eV (Bulb)
18 - 100 keV (SYNCHROTRON)
* 6-7 eV (LASER)

- A QUASIMOMENTUM (

$$\vec{q}_{//} = \vec{q}_{i\,//} - \vec{q}_{e\,//} + \vec{G}_{//}$$

- I/E REMOVE ONE ELECTRON

INDEPENDENT ELECTRON INTERPRETATION



EMITED ELECTRON LEAVES A HOLE

WITH MOMENTUM $\vec{q}_{//} = \vec{q}_{i//} - \vec{q}_{e//} + \vec{G}_{//}$

AND BAND ENERGY $\vec{\mathcal{E}}_{\vec{q}_{//}} = E_e - E_i + E_W$ (WORK-FUNCTION CONSTANT)

WHERE $\mathcal{E}_F = 0$

IN THIS PICTURE WE PROBE THE OCCUPIED ENERGY BANDS

TRUE IN A INDEP-PARTICLE PICTURE

DO WE SEE BANDS? (DOES BLOCH-THEOREM WORK?)

WHY IN PRESENCE OF A HUGE e-e INTERACTION (SIMILAR TO THE e-NUCLEOUS INTERACTION) WE SEE BANDS?

- ELECTRONS MOVE IN AN "EFFECTIVE" ONE BODY POTENTIAL" GENERATED BY NUCLEAI AND BY OTHER ELECTRONS

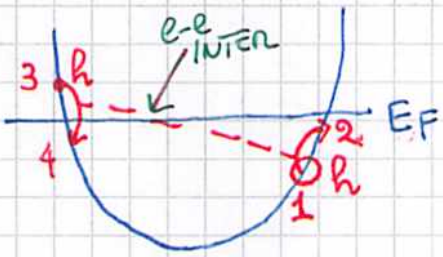
  COMPARABLE SIZE

- WE CAN DEFINE IN A RIGOROUS WAY SUCH "EFFECTIVE POTENTIAL" AND COMPUTE IT NUMERICALLY
  - DIFFERENT APPROACHES (DIFFERENT POTENTIAL)
  - FOR TOTAL ENERGY HF (LOW ACCURACY)
    DFT (HIGH ACCURACY)
  - FOR BAND STRUCTURE DFT (MEDIUM ACCURACY)
    GW (HIGH ACCURACY)

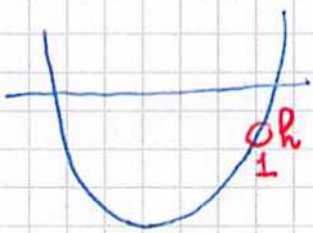
IN THE SLIDES COMPARISON BETWEEN DFT AND ARPES (DFT FOR GRAPHENE RESCALING ~ 15% REQUIRED)

SIGNATURE OF ELECTRON-ELECTRON INTERACTION

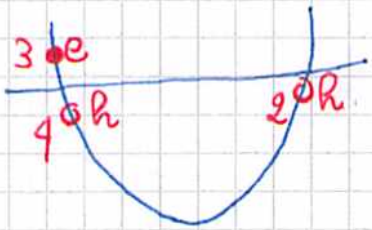
DECAY OF A HOLE (SAME FOR ELECTRON BUT ARPES CREATES HOLES!)



INITIAL STATE



FINAL STATE



CONSERVATION OF ENERGY AND QUASI MOMENTUM BY e-e INTER.

ENERGY $\overbrace{-\varepsilon_{\vec{k}_1}}^{\text{INITIAL}} = \overbrace{-\varepsilon_{\vec{k}_2} - \varepsilon_{\vec{k}_4} + \varepsilon_{\vec{k}_3}}^{\text{FINAL}}$

QUASI-MOMENTUM $-\vec{k}_1 = -\vec{k}_2 - \vec{k}_4 + \vec{k}_3 + \vec{G}$ ← ARBITRARY REC LATTICE VECTOR (INCLUDING $\vec{G}=0$)

BROADENIG OF BAND AT $\vec{k}_1$ BY ARPES

$$\frac{\Gamma_{k_1}}{\hbar} = \frac{1}{\tau_{h_1}} = \frac{2\pi}{\hbar} \int \frac{d^3k_2}{(2\pi)^3} \frac{d^3k_3}{(2\pi)^3} \frac{d^3k_4}{(2\pi)^3} \delta\left(-\varepsilon_{\vec{k}_1} + \varepsilon_{\vec{k}_2} + \varepsilon_{k_4} - \varepsilon_{\vec{k}_3}\right) \times \sum_{\vec{G}} \delta\left(-\vec{k}_1 + \vec{k}_2 + \vec{k}_4 - k_3 + \vec{G}\right) \times \left(\text{MATRIX ELEMENT}\right)^2$$

τ_{h_1}: LIFETIME OF HOLE

$\varepsilon_{\vec{k}_2} < \varepsilon_F$

$\varepsilon_{\vec{k}_4} < \varepsilon_F$

$\varepsilon_{\vec{k}_3} > \varepsilon_F$

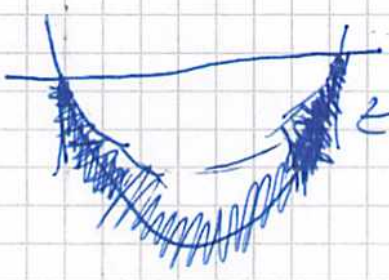
[FERMI GOLDEN RULE $\Gamma_i = \frac{2\pi}{\hbar} \sum_f |\langle f|H^{(1)}|i\rangle|^2 \delta(\varepsilon_f - \varepsilon_i)$] :

AT = 0 IN 3D (FOR BOTH HOLES AND ELECTRONS)

$$\Gamma_{k_1} \propto (\varepsilon_F - \varepsilon_{\vec{k}_1})^2$$

IN 2D

$$\Gamma_{k_1} \propto (\varepsilon_F - \varepsilon_{\vec{k}_1})^2 \ln\left(\frac{\varepsilon_F}{|\varepsilon_F - \varepsilon_{k_1}|}\right)$$

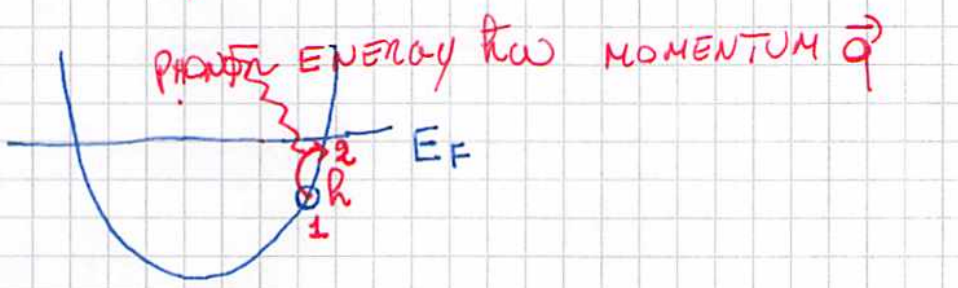


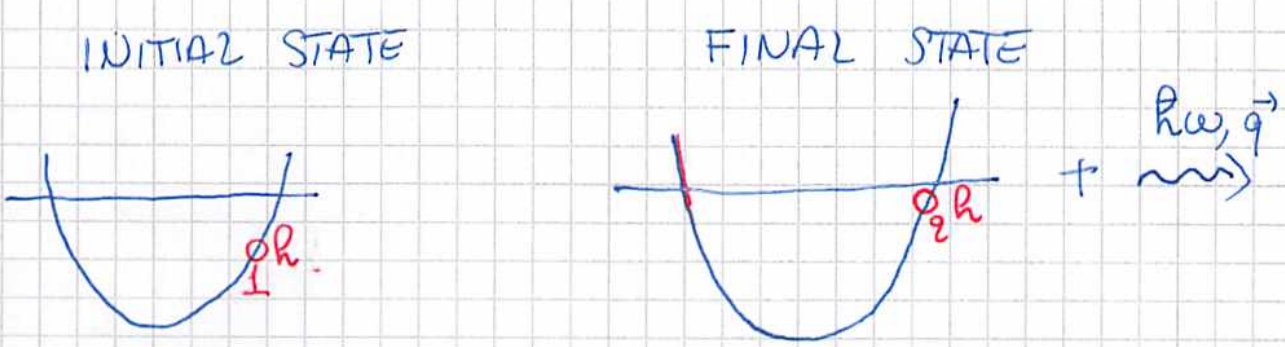
← BROADENING INCREASES WITH THE DISTANCE FROM THE FERMI ENERGY

SIGNATURE OF ELECTRON-PHONON INTERACTION

DECAY OF A HOLE INTO A NON-DISPERSIVE OPTICAL PHONON (EINSTEIN-MODE)

$\hbar\omega_{\vec{q}} = \hbar\omega$





CONSERVATION OF ENERGY

$$-\varepsilon_{\vec{k}_1} = -\varepsilon_{\vec{k}_2} + \hbar\omega$$

ONLY POSSIBLE IF $(\varepsilon_F - \varepsilon_{\vec{k}_1}) > \hbar\omega$

CONSERVATION OF MOMENTUM

$$-\vec{k}_1 = -\vec{k}_2 + \vec{q} + \vec{G}$$

$\vec{G} \in$ RECIPROCAL LATTICE

IF $\vec{G} = 0$ $\quad \vec{q} = \vec{k}_2 - \vec{k}_1$

FERMI GOLDEN RULE

$$\frac{\Gamma_{\vec{k}_1}}{\hbar} = \frac{1}{\tau_{\vec{k}_1}} = \frac{2\pi}{\hbar} \int_{\varepsilon_{\vec{k}_2} < \varepsilon_F} \frac{d^3k_2}{(2\pi)^3}\, \delta\left[\varepsilon_{\vec{k}_2} - \left(\varepsilon_{\vec{k}_1} + \hbar\omega\right)\right] M^2$$

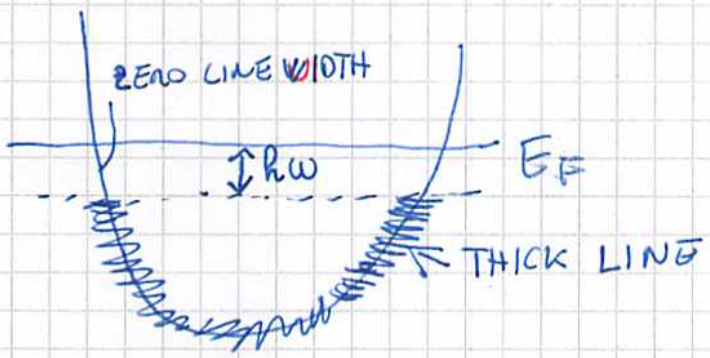
IF M^2 INDEPENDENT OF $\vec{k}_1, \vec{k}_2$

$$\Gamma_{\vec{k}_1} = 2\pi M^2 \int_{\substack{\varepsilon_F - \varepsilon_{\vec{k}_1} > \hbar\omega}} \frac{d^3k_2}{(2\pi)^3} \delta\left[\varepsilon_{\vec{k}_2} - (\varepsilon_{\vec{k}_1} + \hbar\omega)\right]$$

$$= 2\pi M_x^2 \begin{cases} 0 \quad \text{IF } \varepsilon_F - \varepsilon_{k_1} < \hbar\omega \\ \frac{1}{2} \, DOS(\varepsilon_{k_1} + \hbar\omega) \end{cases}$$

SPIN

ELECTRONIC DENSITY OF STATES



OTHER DECAYS (PLASMON, SCATTERING ON DEFECTS...)

UNITS

GAUSSIAN UNITS $[Q] = \text{STATC}$

COULOMB LAW $F = \frac{Q_1 Q_1}{r^2}$ $\quad [\vec{E}] = [\vec{B}]$

ATOMIC UNITS

$m_e = 1 \quad \hbar = 1 \quad e = 1 \quad \therefore \alpha = \text{FINE STRUCTURE CONSTANT} = \frac{e^2}{\hbar c} \approx \frac{1}{137}$

$\Downarrow$

$c = 137$

$[\text{ENERGY}] = \text{HARTREE} = 2\,\text{Rydberg} = 2 \times (13.605\ \text{eV})$

$[\text{length}] = a_0 = \frac{\hbar^2}{m_e e^2} = \text{BOHR RADIUS} = 0,529177\ \text{Å}$

HAMILTONIAN $\vec{B}=0$

$$H = \sum_i H_i^{1e} + \sum_{\substack{ij \\ j\neq i}} H_{ij}^{2e}$$

$$H_i^{1e} = \frac{1}{2m_e} p_i^2 + V(\vec{r}_i) + \underbrace{\frac{1}{2}\frac{1}{(m_e c)^2}\vec{\nabla}\cdot V(r_i) \times \vec{p}_i \cdot \vec{S}_i}_{\text{SPIN ORBIT}}$$

$$S_z|\uparrow\rangle = \frac{1}{2}\hbar|\uparrow\rangle$$

$$H_{ij}^{2e} = \frac{1}{2}\frac{e^2}{|\vec{r}_i - \vec{r}_j|} \underbrace{- \frac{1}{2}\frac{1}{(m_e c)^2}\frac{\vec{r}_i - \vec{r}_j}{|\vec{r}_i - \vec{r}_j|^3} \times \vec{p}_i \cdot \vec{S}_i}_{\text{SPIN. ORBIT}}$$

SPIN-ORBIT HEURISTIC DERIVATION

ELECTRIC FIELD $\vec{E} = +\frac{\vec{\nabla} V(\vec{r})}{e}$

ELECTRON VELOCITY $= \frac{\vec{p}}{m_e}$

EFFECTIVE $\vec{B}$ FIELD IN THE REFERENCE FRAME OF ELECTRON

$$\vec{B} = -\frac{\vec{v}}{c} \times \vec{E} = \frac{1}{m_e c e} \vec{\nabla} V \times \vec{p}$$

$$H_H^{so} = g_s \frac{\mu_B}{\hbar} \vec{S} \cdot \vec{B} \qquad g_s \sim 2 \qquad \mu_B = \frac{e\hbar}{2 m_e c}$$

$$H^{so} = \left(\frac{1}{2}\right) H_H^{so} = \frac{g_s}{2} \frac{1}{\hbar m_e c} \frac{e\hbar}{2 m_e c} = \frac{g_s}{4} \frac{1}{m_e^2 c^2} \vec{\nabla} V \times \vec{p} \cdot \vec{S}$$

→ THOMAS PRECESSION

$$g_s \simeq 2 \qquad H^{so} = \frac{1}{2 m_e^2 c^2} \left(\vec{\nabla} V \times \vec{p}\right) \cdot \vec{S}$$

• NOTATIONS

• ONE ELECTRON

DIRAC

$|\overline{a}\rangle \in \{$SPACIAL SPACE $\otimes$ SPIN SPACE$\}$ FOR BREVITY

$|\overline{\vec{r},s}\rangle = |\vec{r}\rangle \otimes |s\rangle = |\vec{r},s\rangle \quad \vec{r} \in 3\mathbb{R}$

$s = \uparrow, \downarrow = 1, -1$

$S_z|s\rangle = \frac{\hbar}{2} s |s\rangle$

SCHRÖDINGER

$\psi(\vec{r},s) \equiv \langle \vec{r},s|\overline{A}\rangle$

OR $\psi_s(\vec{r}) \equiv \psi(\vec{r},s)$

SPINOR NOTATION (2 COMPONENT VECTOR)
SCHRODINGER DIRAC

$$\begin{pmatrix} \psi(\vec{r},\uparrow) \\ \psi(\vec{r},\downarrow) \end{pmatrix} \equiv \overline{\psi}(\vec{r})$$

• SIMPLIFIED SITUATION : FACTORIZED SPIN

IN ABSENCE OF SPIN-ORBIT

$[S_z, H] = 0$

↓

$\exists$ - SPIN-FACTORIZED EIGEN-STATES OF H

$\overline{|a\rangle} = |a\rangle \otimes |s\rangle$ IN SPINOR EITHER $\begin{pmatrix} \psi(z) \\ 0 \end{pmatrix}$ OR $\begin{pmatrix} 0 \\ \psi(z) \end{pmatrix}$

NOT TRUE IN PRESENCE OF SPIN-ORBIT

WITHIN A MEAN-FIELD APPROACH (SEE LATER)
INDIVIDUAL ELECTRONS IN THE SYSTEM - GROUND STATE
CAN BE SPINOR INSTEAD OF SPIN-FACTORIZED
EVEN IN ABSENCE OF SPIN-ORBIT

IN PARTICULAR - NON-MAGNETIC-N-ELECTRONS
FOR ANY AXIS : SPIN FACTORIZED

- MAGNETIC SYSTEMS
  - COLINEAR FERROMAGNETISM
    ANTI FERROMAGNETISM

    SPIN-FACTORIZED
    WITH $\hat{z}$ // MAGNETISATION
  - NON-COLINEAR MAGNETISM

    SPIN - CAN NOT BE FACTORIZED
    ELECTRON SHOULD BE REPRESENTED
    WITH SPINORS

KRAMER'S DOUBLET

EVEN IN PRESENCE OF SPIN ORBIT THE HAMILTONIAN IS INVARIANT UNDER TIME REVERSAL

T = TIME REVERSAL OPERATOR

$$T^2 = -1 \qquad T^{-1} = -T$$

$$T^{-1}\vec{r}\,T = \vec{r} \qquad T^{-1}\vec{p}\,T = -\vec{p} \qquad T^{-1}\vec{S}\,T = -\vec{S}$$

IN SCHRÖDINGER REPRESENTATION

$$T = -i\sigma_y\,CC = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} CC$$

CC ↓ complex conjugate

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\Downarrow$$

$$T^{-1}H\,T = H$$

$$H^{1e}\,|\bar{a}\rangle = E_a\,|\bar{a}\rangle$$

$$T^{-1}H^{1e}T\,|\bar{a}\rangle = E_a\,|\bar{a}\rangle$$

$$H^{1e}T\,|\bar{a}\rangle = E_a\,T\,|\bar{a}\rangle$$

$$H^{1e}\,|\bar{a}'\rangle = E_a\,|\bar{a}'\rangle \qquad |a'\rangle = T|\bar{a}\rangle$$

$\{|\bar{a}\rangle, |\bar{a}'\rangle\}$ DEGENERATE KRAMER'S DOUBLET WITH EIGENENERGY E_a

NOTE THAT $|\alpha'\rangle$ AND $|\alpha\rangle$ DISTINCT STATES

SINCE $\langle \vec{r}|\bar{\alpha}\rangle = \begin{pmatrix}\psi(\vec{r},\uparrow)\\ \psi(\vec{r},\downarrow)\end{pmatrix}$

$$\langle \bar{\alpha}|\bar{\alpha}'\rangle = \langle \bar{\alpha}^T \bar{\alpha}\rangle = \int d^3r \left(-\psi^*(\vec{r},\uparrow)\psi^*(\vec{r},\downarrow) + \psi^*(\vec{r},\downarrow)\psi^*(\vec{r},\uparrow)\right)$$

$$= 0$$