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SMR. 628 - 27

Research Workshop in Condensed Matter,
Atomic and Molecular Physics
(22 June - 11 September 1992)

Working Party on:
"Energy Transfer in Interactions with
Surfaces and Adsorbates"
(31 August - 11 September 1992)

"Stopping Power and Charge Transfer"
for light ions (He) in (or near) metals

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These are preliminary lecture notes, intended only for distribution to participants.

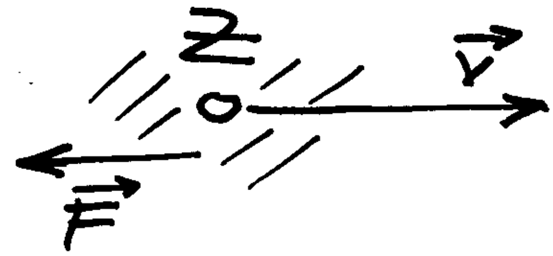
Stopping power

and

charge transfer

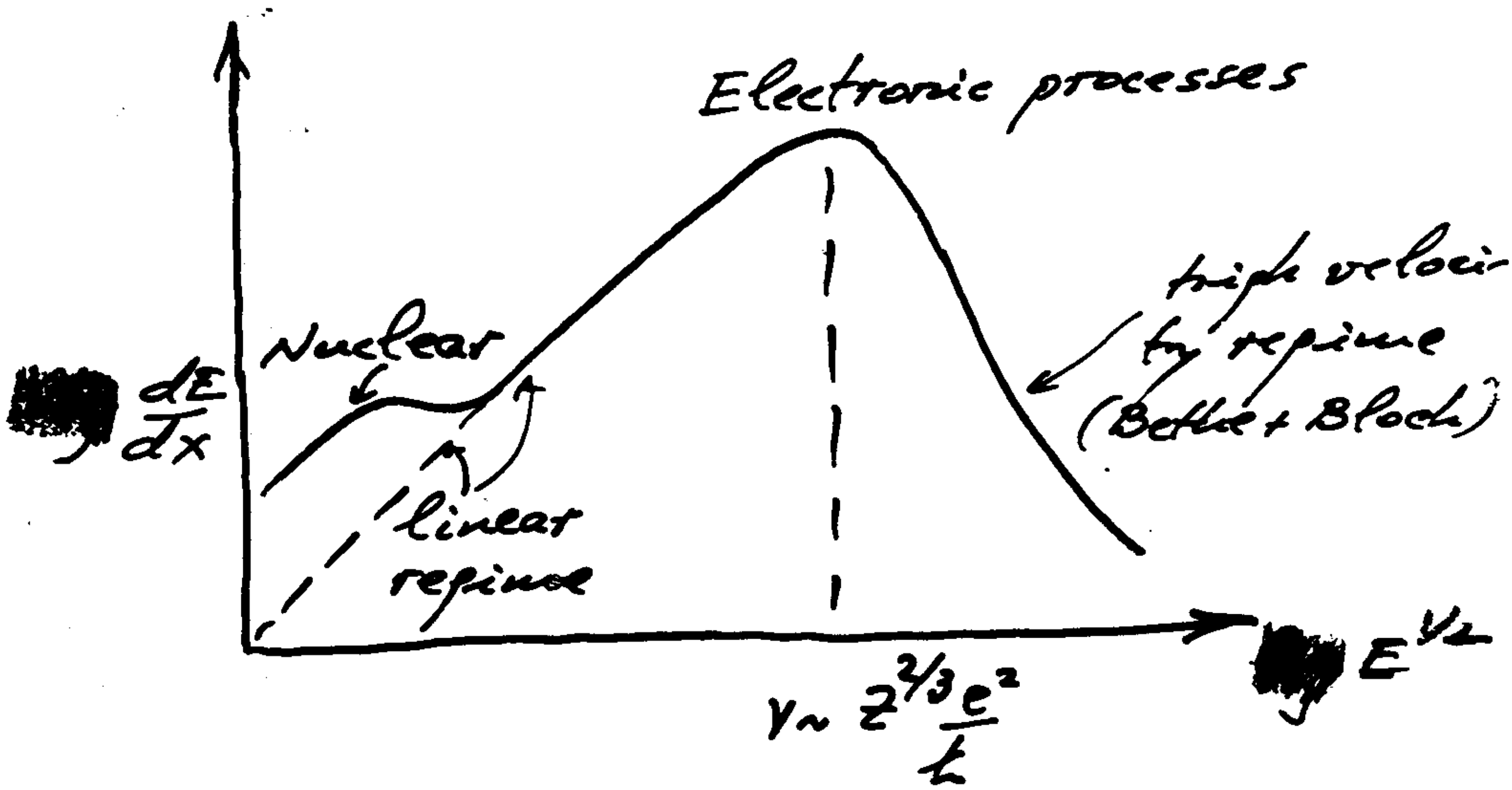
for light ions (He)
in (or near) metals

2. General considerations



Stopping power

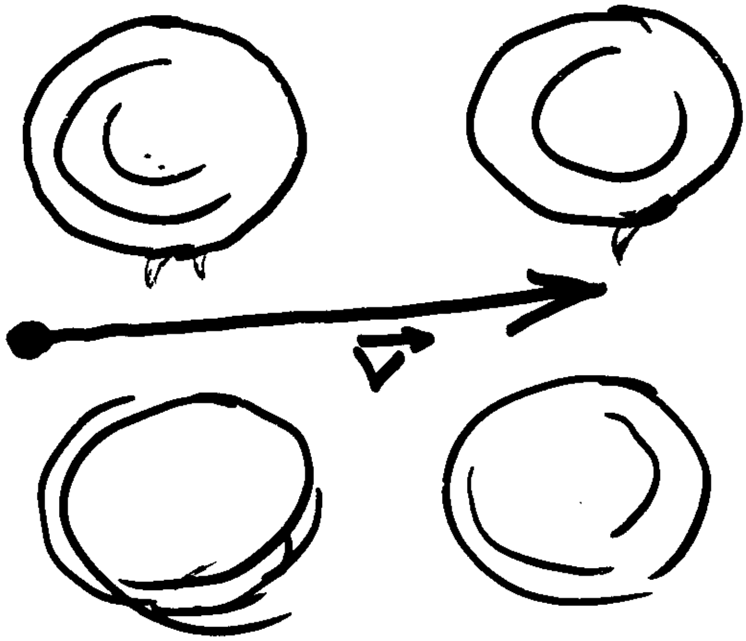
Bohr (1913), Bethe (1930), Bloch (1933)



$v \ll Z^{2/3} \frac{e^2}{\hbar}$ linear regime

$v \sim Z^{2/3} \frac{e^2}{\hbar}$ intermediate regime

$v \gg Z^{2/3} \frac{e^2}{\hbar}$ high velocity limit



Lindhard, Sigmund, Ritchie, Echenique et al....

Linear Response Theory

Kinetic theory

LDA

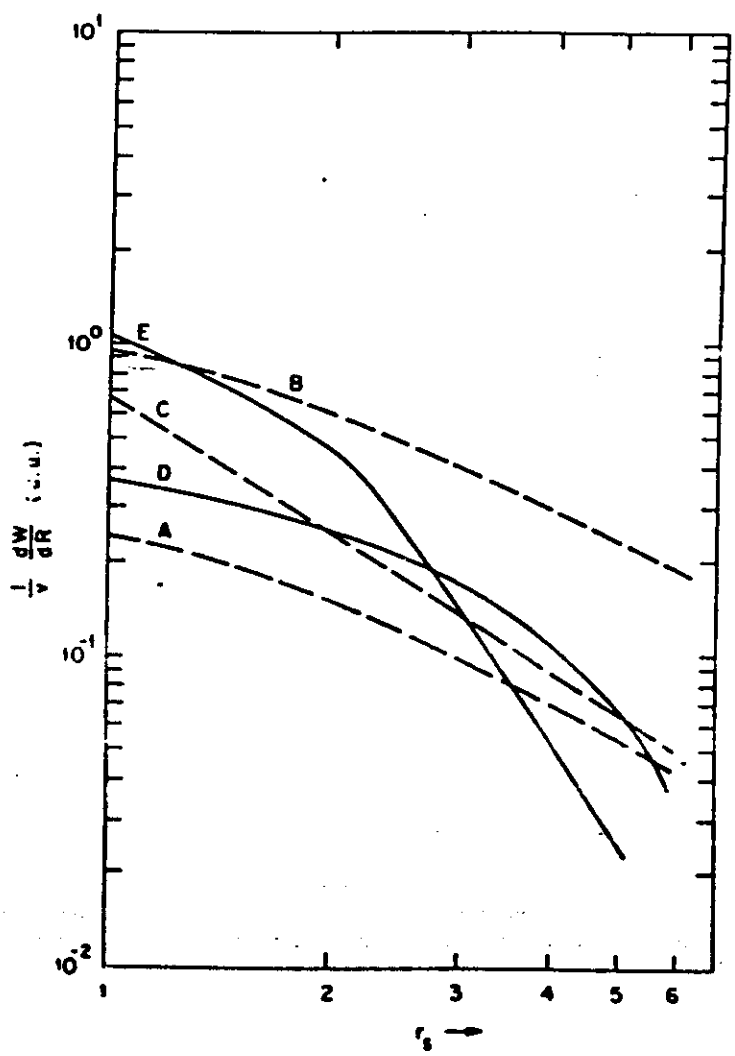


FIG. 12. Stopping powers as functions of r_s. Curve A is calculated in linear response theory, Eq. (26.1), for $Z_1 = 1$; curve B from Eq. (26.1) with $Z_1 = 2$. Curve C is the result Ferrell and Ritchie from (Ref. 102) for a slow, singly ionized He atom. Curves D and E are the density functional results for a proton and a helium nucleus, respectively. In all cases $v \ll v_F$.

[redacted] $v \sim z^{2/3} \, \varepsilon/t$

Intermediate velocity

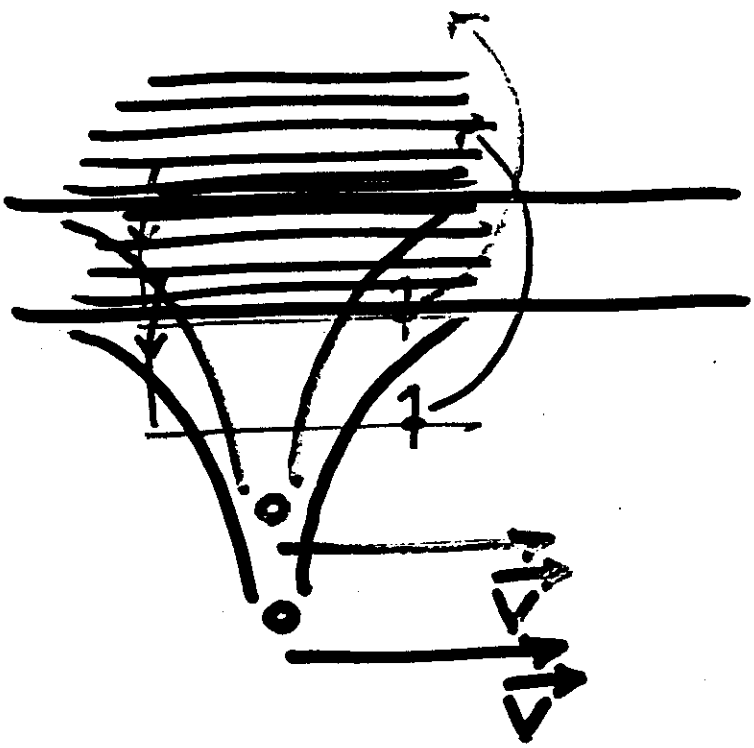
Intermediate velocity

$$z^* = z\left(1 - e^{-\frac{v_0}{v} z^{2/3}}\right)$$

$$z^* = z\left(1 - e^{-\frac{v}{v_0 z^{2/3}}}\right)$$

Brandt and coworkers

Brandt and coworkers



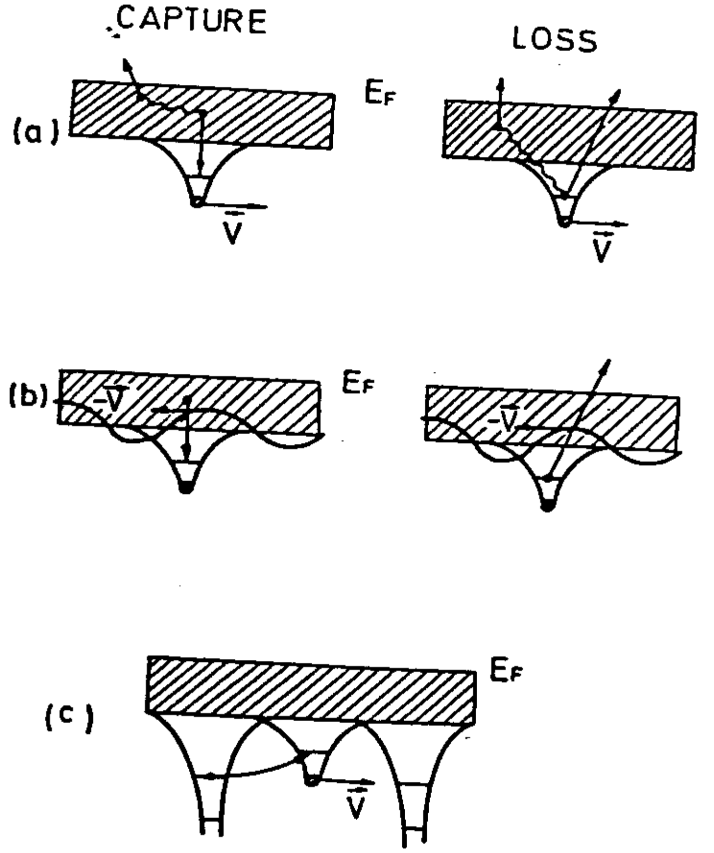


FIG. 19. (a) Shows an Auger process for an ion moving in a uniform electron gas: (i) a conduction electron jumps to a bound state on the ion, (ii) an electron bound to the ion is excited to the conduction band. (b) Shows the coherent resonant process for an ion moving in a crystal: (i) in a capture process, the crystal pseudopotential induces transitions between a conduction and a bound state; (ii) in a loss process, an electron bound to the ion is excited to a level of the conduction band. (c) Illustrates the shell process whereby an ion moving in crystal captures one electron from an inner level of the target.

Echenique, F + Ritchie
Solid State Physics
...ries 43 (1989)

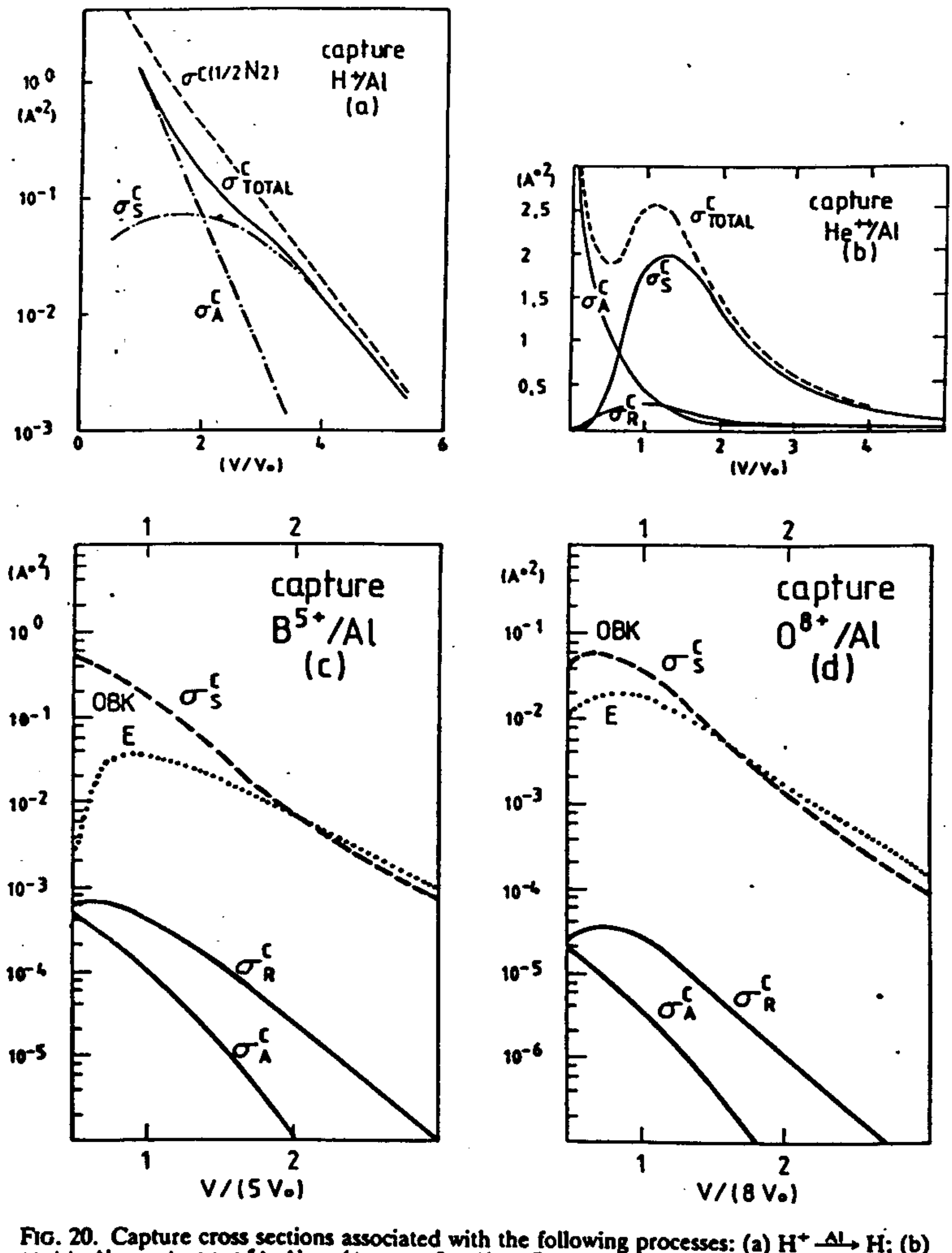


FIG. 20. Capture cross sections associated with the following processes: (a) $H^+ \xrightarrow{Al} H$; (b) $He^{++} \xrightarrow{Al} He^+$; (c) $B^{5+} \xrightarrow{Al} B^{4+}$; (d) $O^{8+} \xrightarrow{Al} O^{7+}$. Shell ($\sigma_s$) Auger ($\sigma_A$) and resonant ($\sigma_R$) processes are shown. For H, the resonant process is unimportant; also shown is the cross section for the atomic collision $H^+ \xrightarrow{N_2} H$, normalized to one N atom. For B and O, the shell cross sections calculated using an OBK approximation and an eikonal (E) approach are given.

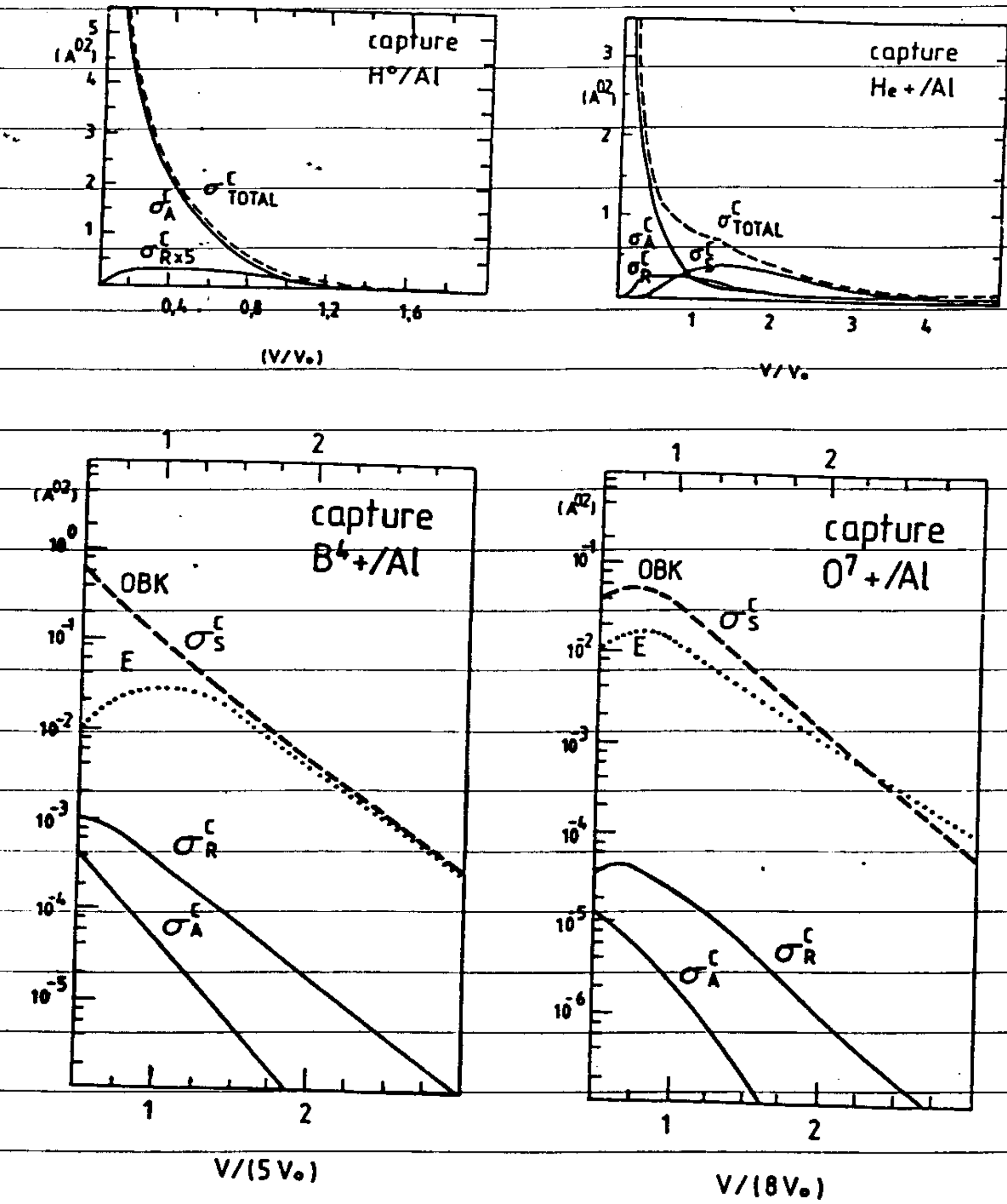


FIG. 21. As in Fig. 20 for (a) $H \xrightarrow{Al} H^-$; $He^+ \xrightarrow{Al} He$, (c) $B^{4+} \xrightarrow{Al} B^{3+}$ and (d) $O^{7+} \xrightarrow{Al} O^{6+}$.

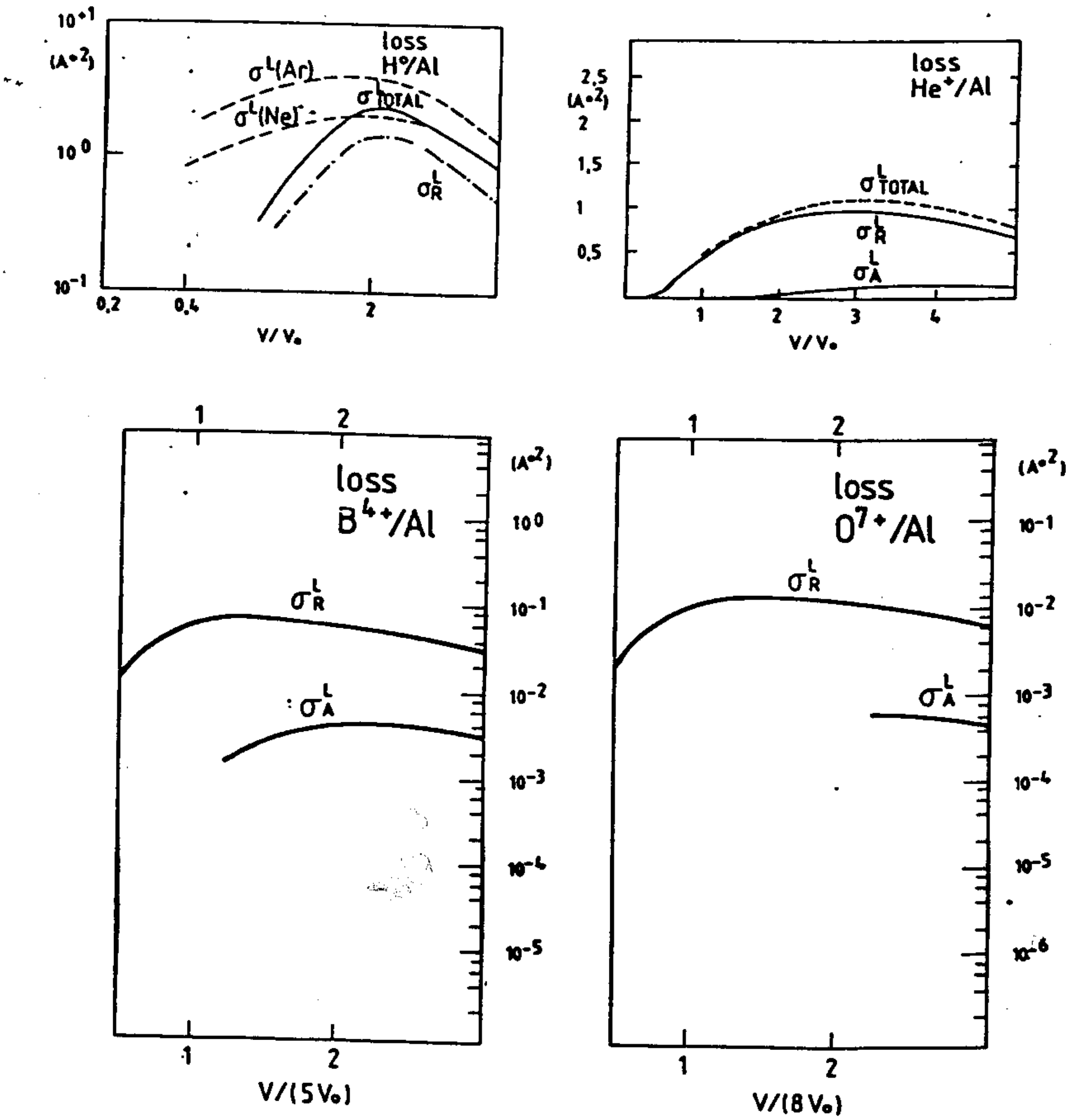


FIG. 22. Loss cross sections associated with the following processes: (a) $H \xrightarrow{Al} H^+$, (b) $He^+ \xrightarrow{Al} He^{++}$, (c) $B4^+ \xrightarrow{Al} B^{5+}$, (d) $O^{7+} \xrightarrow{Al} O^{8+}$. Auger ($\sigma_A$) and resonant ($\sigma_R$) processes are shown. For H, the cross sections for the atomic collisions $H^0 \xrightarrow{Ar} H^+$ and $H^0 \xrightarrow{Ne} H^+$ are also shown.

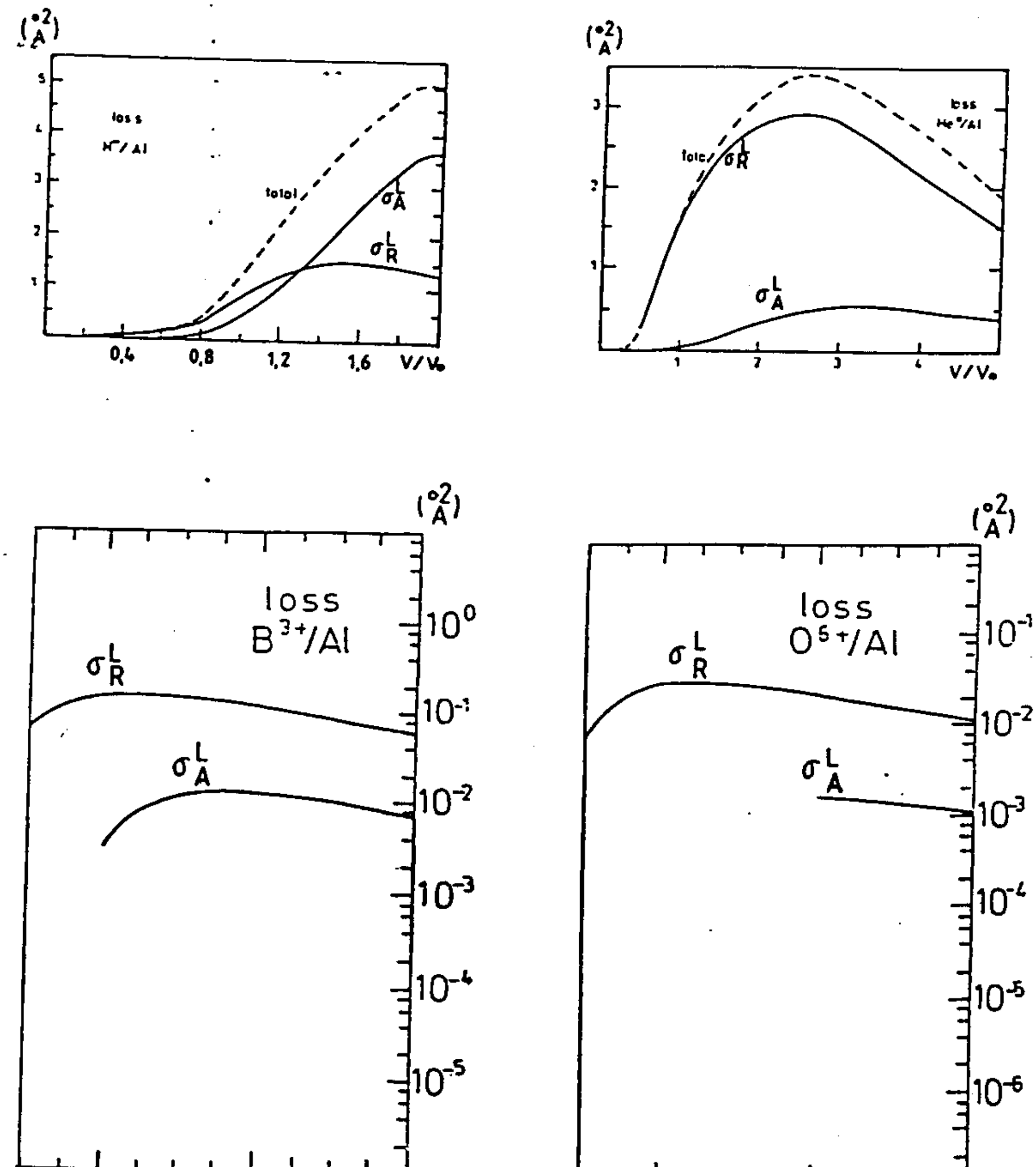


FIG. 23. As in Fig. 22 for (a) $H^- \xrightarrow{Al} H$, (b) $He^0 \xrightarrow{Al} He^+$, (c) $B^{3+} \xrightarrow{Al} B^{4+}$, and (d) $O^{6+} \xrightarrow{Al} O^{7+}$.

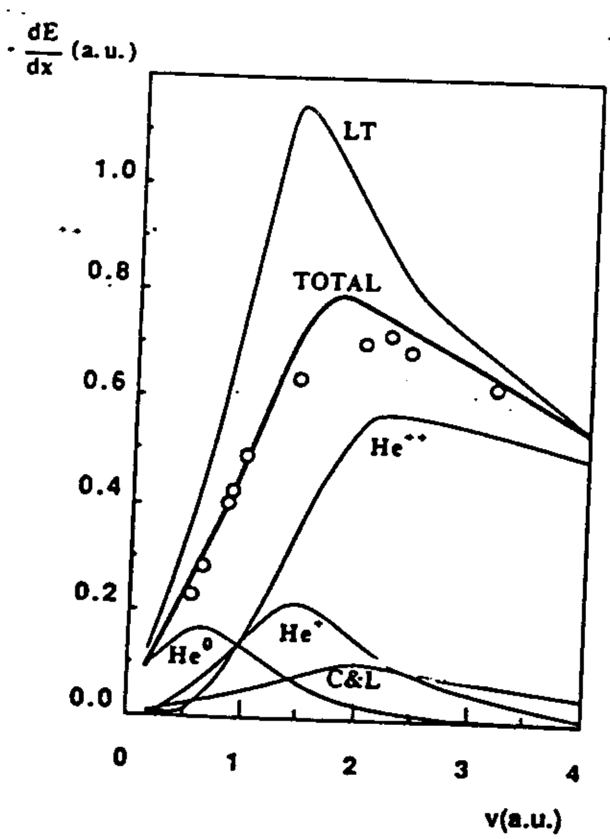


FIG. 1. Stopping power in atomic units of Al for helium ions as a function of ion speed. The thick solid line (TOTAL) is the result of our calculation and the curve labeled LT is obtained from linear-response theory for a bare ion. Both of them include inner-shell corrections. The circles are the experimental data. The different contributions to the curve labeled TOTAL from the fractions of bare ions (He^{++}), singly ionized ions (He^{+}), neutral atoms (He^{0}), and capture and loss processes (C&L) are shown separately.

Peñalva et al
Phys. Rev. Lett. (1986)

$$\frac{dE}{dx} = n^{0}\,\frac{dE}{dx}(He^{0}) + n^{+}\,\frac{dE}{dx}(He^{+})$$

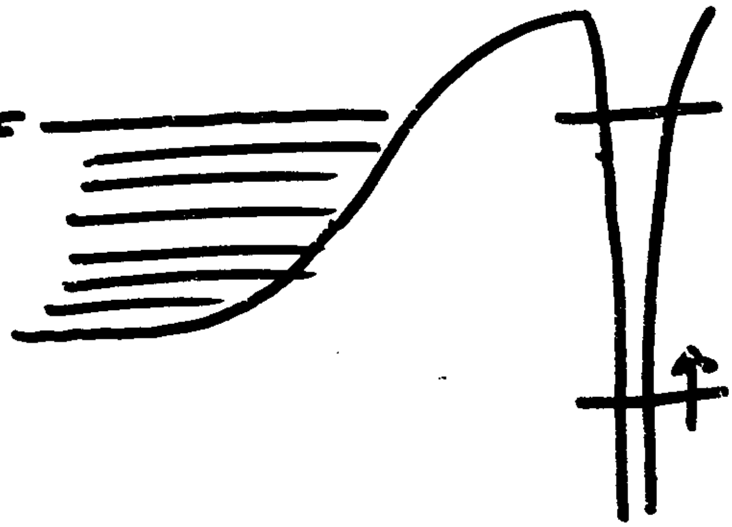
$$+\, n^{++}\,\frac{dE}{dx}(He^{++})$$

$$+ \left(\frac{dE}{dx}\right)_{\text{Capture + Loss}}$$

General considerations

1. Ions approaching surfaces

E_F



He^+ or He^*

(a) Chemisorption: Li, Na, K ....

(b) Charge transfer: resonance and Auger processes

Norlander Ziman ..., Heiland + Taglauer

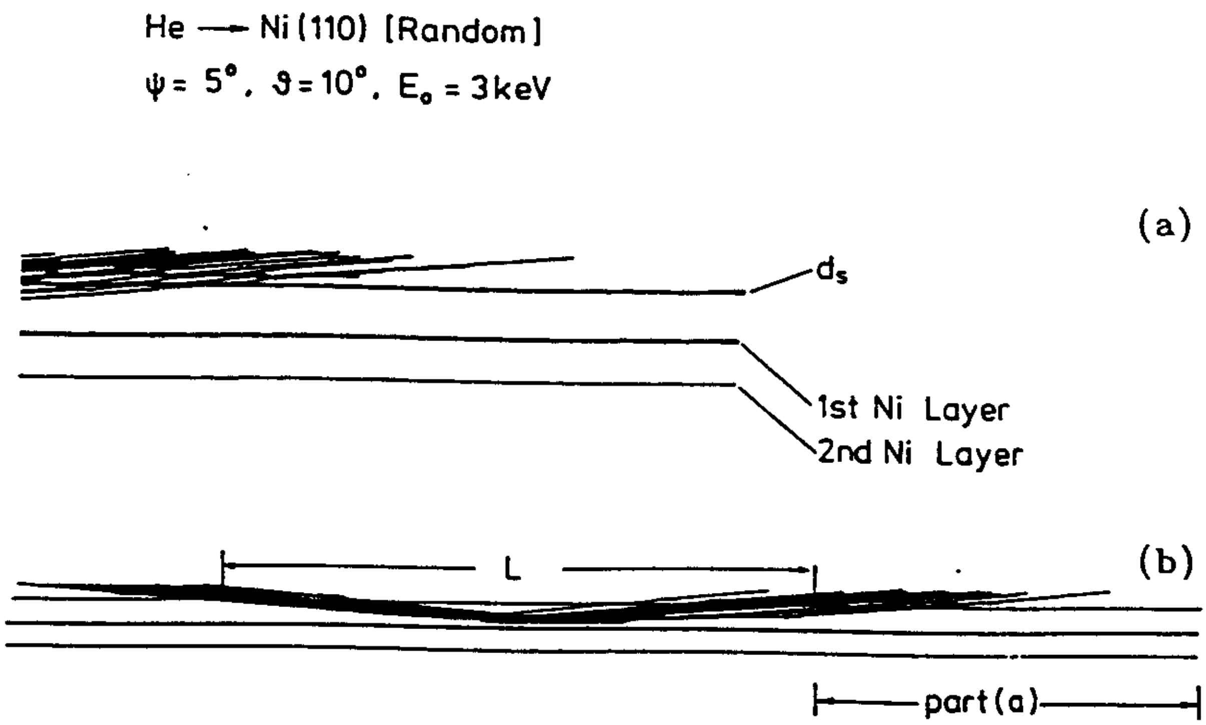


FIG. 11. Sketch of how the trajectory length L was determined from the MARLOWE data. The obtained values are listed in Table III.

Narmann et al
PRL (1989)

Dynamic interaction of

Dynamic interaction of ions

ions ~~with condensed matter~~

with condensed matter using

using a LCAO approach

a LCAO approach

C. Monreal, J.J. Dorado

C. Monreal, F.J. Garcia-Vidal, J. Ortega,

F. J. Garcia-Vidal, J. Ortega

J. Dorado and N. Lorente

N. Lorente and F. Flores

Why an LCAO approach?

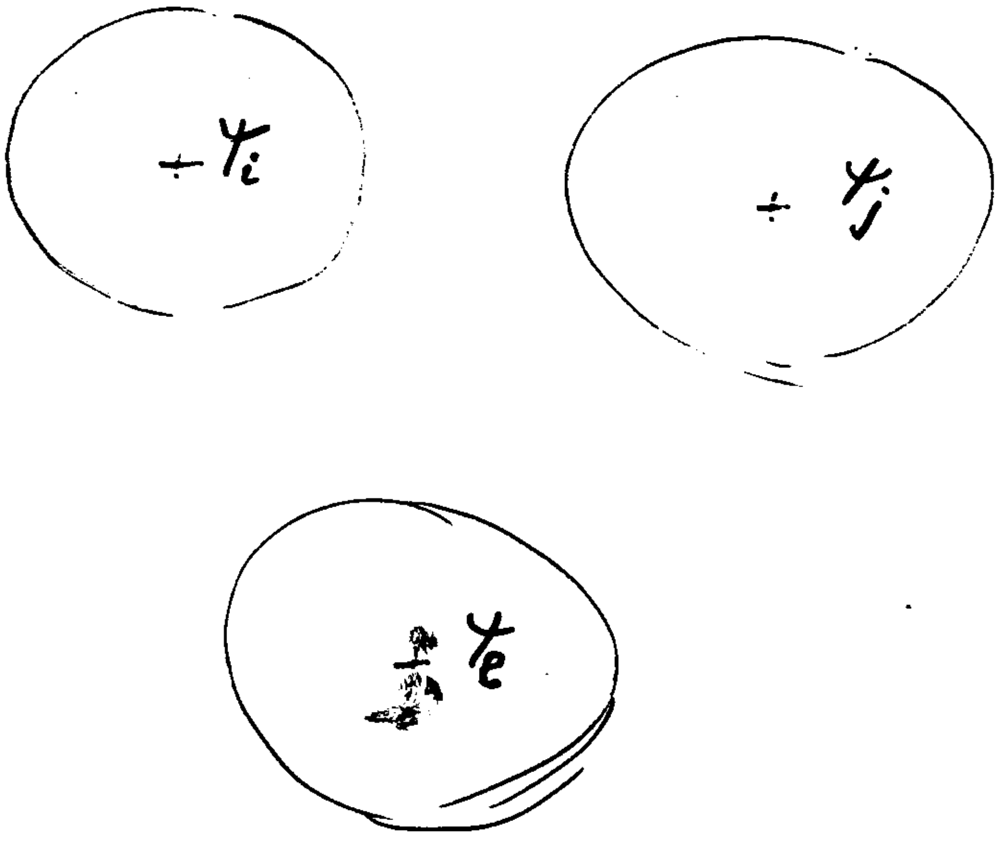
(a) Our first motivation: apply to this field an ab-initio LCAO method we have developed for calculating electronic properties of solids

(b) Second reason: to calculate the stopping power of ions in __inhomo__-__geneous__ __systems__ → surfaces, transition metals (d-bands) etc.
+ charge transfer near ~~[illegible]~~ (+)

charge transfer processes near surfaces including the atomic structure

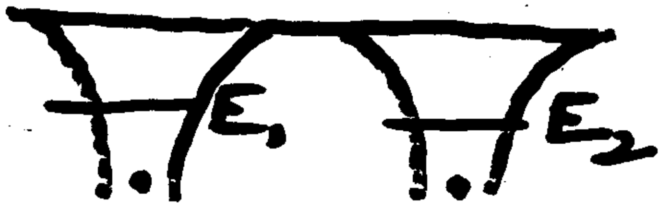
LCAO-method for calculating the electronic properties of solids

PRB 44, 11412 (91)



$\psi \equiv$ atomic wavefunctions

H_2^+



$$\hat{H} = -\tfrac{1}{2}\nabla^2 - \frac{1}{|\mathbf{r}-\mathbf{R}_1|} - \frac{1}{|\mathbf{r}-\mathbf{R}_2|} + \frac{1}{d} , \qquad (22)$$

Atomic wavefunctions

$$\psi_1(\mathbf{r}) = (\alpha^3/\pi)^{1/2} e^{-\alpha|\mathbf{r}-\mathbf{R}_1|} , \qquad (23a)$$

$$\psi_2(\mathbf{r}) = (\beta^3/\pi)^{1/2} e^{-\beta|\mathbf{r}-\mathbf{R}_2|} . \qquad (23b)$$

Lowdin's wavefunctions

$$\phi_1(\mathbf{r}) = \lambda\psi_1 + \mu\psi_2 , \qquad (24a)$$

$$\phi_2(\mathbf{r}) = \mu\psi_1 + \lambda\psi_2 , \qquad (24b)$$

where $\lambda = (1/\sqrt{1+S} + 1/\sqrt{1-S})/2$ and $\mu = (1/\sqrt{1+S} - 1/\sqrt{1-S})/2$, S being the overlap between orbitals ψ_1 and ψ_2.

2nd quantization Hamiltonian

$$\hat{H} = \sum_\sigma (\varepsilon_1 n_{1\sigma} + \varepsilon_2 n_{2\sigma})$$
$$+ t \sum_\sigma (C^\dagger_{1\sigma} C_{2\sigma} + C^\dagger_{2\sigma} C_{1\sigma}) + 1/d \ , \qquad (25)$$

where

$$\varepsilon_i = \int \phi_i \left[-\tfrac{1}{2}\nabla^2 - \frac{1}{|\mathbf{r}-\mathbf{R}_1|} - \frac{1}{|\mathbf{r}-\mathbf{R}_2|} \right] \phi_i \, d\mathbf{r} \qquad (26a)$$

and

$$t = \int \phi_1 \left[-\tfrac{1}{2}\nabla^2 - \frac{1}{|\mathbf{r}-\mathbf{R}_1|} - \frac{1}{|\mathbf{r}-\mathbf{R}_2|} \right] \phi_2 \, d\mathbf{r} \ . \qquad (26b)$$

$$\varepsilon_i = \varepsilon_i^0 - \tfrac{1}{2}[1-(1-S^2)^{1/2}](\varepsilon_j^0 - \varepsilon_i^0) - St \ , \qquad (27a)$$

$$t = -\frac{1}{1-S^2}\frac{S}{2}(\varepsilon_1^0 + \varepsilon_2^0) + \frac{1}{1-S^2} t^0 \ , \qquad (27b)$$

$$\varepsilon_i^0 = \int \psi_i \left(-\tfrac{1}{2}\nabla^2 + V_1 + V_2\right) \psi_i \, d\underline{r}$$

In many cases, ε_i and t can be obtained with good accuracy by expanding the eqns. for S up to second order in S:

$$\varepsilon_i \simeq \varepsilon_i^{(0)} + \frac{1}{4} S^2 (\varepsilon_i^{(0)} - \varepsilon_j^{(0)}) - S t$$

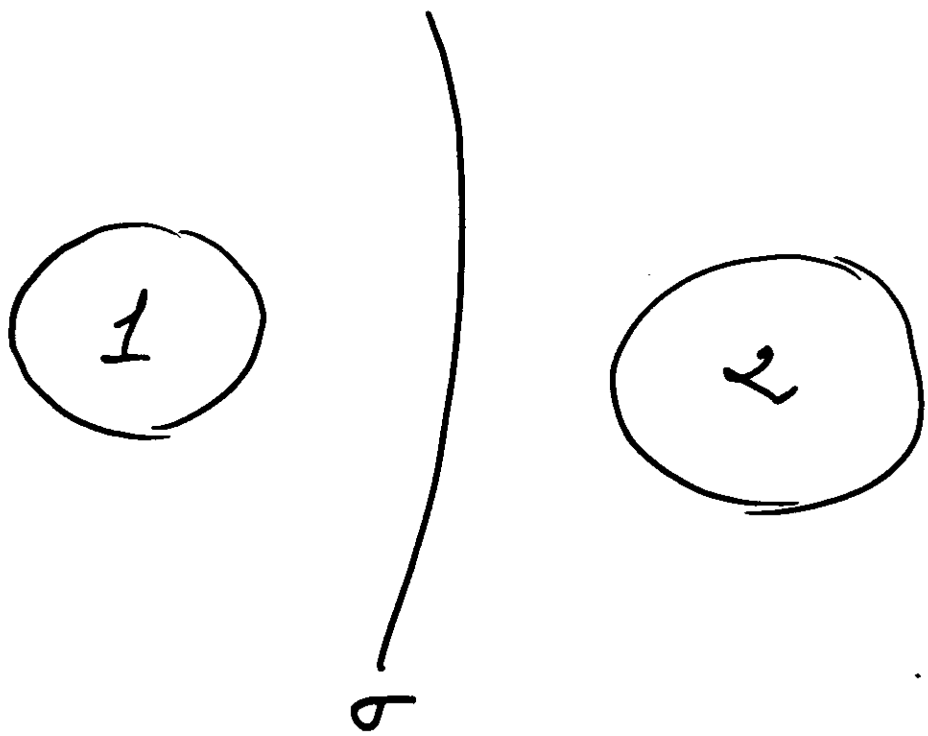
$$t = t^{(0)} \cdot \frac{S}{2} (\varepsilon_i^{(0)} + \varepsilon_j^{(0)})$$

$$- \quad \delta \varepsilon_i = \frac{1}{4} S^2 (\varepsilon_i^{(0)} - \varepsilon_j^{(0)}) - S t$$

is due to the increase in the kinetic energy due to the orbitals overlap

$$-t \simeq \gamma\, t^B$$

$$t^B = -\frac{1}{2}\int_\sigma \left(\psi_1 \vec{\nabla}\psi_2 - \psi_2 \vec{\nabla}\psi_1\right)\cdot \bar{n}\, ds$$



with

$$\frac{1}{2}\int_\Omega \psi_1 \psi_2\, d\underset{\sim}{r} = \int_{\Omega_1} \psi_1 \psi_2\, d\underset{\sim}{r} = \int_{\Omega_2} \psi_1 \psi_2\, d\underset{\sim}{r}$$

In general:

$$\hat{H} = \sum_{i\sigma} E_{i\sigma}\,\hat{n}_{i\sigma} + \sum_{i\neq j,\sigma} T_{ij}\left(c^{+}_{i\sigma} c_{j\sigma} + c^{+}_{j\sigma} c_{i\sigma}\right)$$

$$+ \sum_{i} U_i\,\hat{n}_{i\uparrow}\,\hat{n}_{i\downarrow} + \sum_{ij} J_{ij}\left(n_{i\uparrow} n_{j\downarrow} + \right.$$

$$\left. + \frac{1}{2} n_{i\uparrow} n_{j\uparrow} + \frac{1}{2} n_{i\downarrow} n_{j\downarrow}\right) + \sum_{ij} \frac{Z_i Z_j}{d_{ij}}$$

E_i includes the repulsive kinetic energy

T_{ij} is given by T_{ij}^{B}

U_i and J_{ij} are the coulomb interactions between different electrons

$$\hat{H} = \sum_{i,\sigma} E_{i\sigma} \hat{n}_{i\sigma} + \sum_{\substack{i\neq j \\ \sigma}} T_{ij} (c_{i\sigma}^{+} c_{j\sigma} + c_{j\sigma}^{+} c_{i\sigma}) +$$

$$+ \sum_{i} U_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \frac{1}{2} \sum_{\substack{i\neq j \\ \sigma}} (J_{ij} \hat{n}_{i\sigma} \hat{n}_{j\sigma} +$$

$$+ \tilde{J}_{ij} \hat{n}_{i\sigma} \hat{n}_{j\bar{\sigma}}) + \sum_{i\neq j} \frac{1}{2} \frac{Z_i Z_j}{d_{ij}}$$

$$E_i = \varepsilon_i^{(0)} + \frac{1}{4} \sum_j S_{ij}^2 (\varepsilon_i^{(0)} - \varepsilon_j^{(0)}) - \sum_j S_{ij} T_{ij}$$

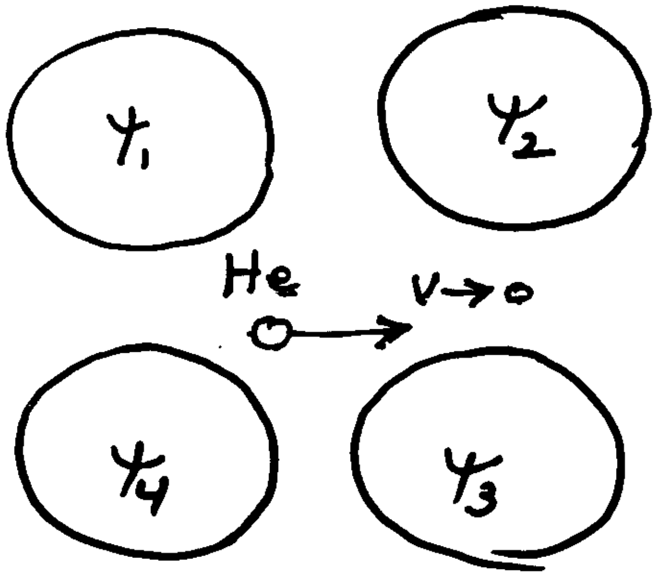
$$T_{ij} = -\frac{\gamma}{2} \int_{\sigma} (\psi_i \vec{\nabla} \psi_j - \psi_j \vec{\nabla} \psi_i) \cdot \vec{n} \, ds$$

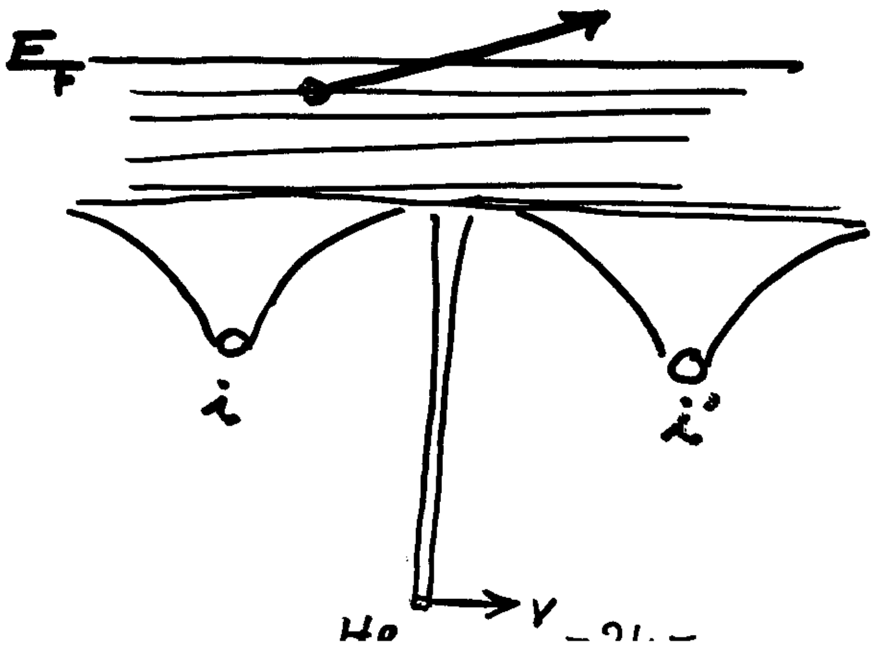
$$S_{ij} = \int \psi_i \psi_j \, d\tau$$

U and J are the coulomb interactions between different electrons

Stopping power for He in metals.
Low velocity limit

Model



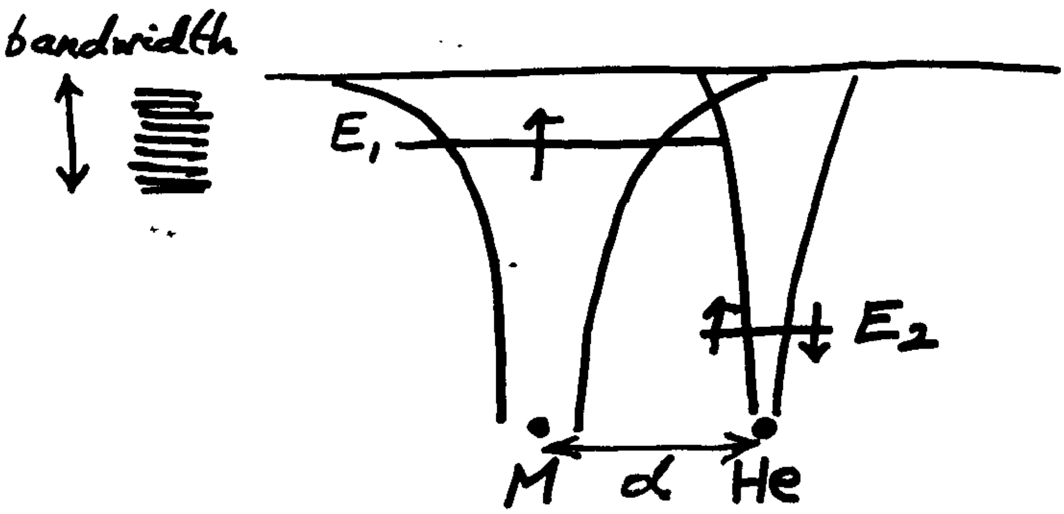


Conduction band

(Li, Na, K...)

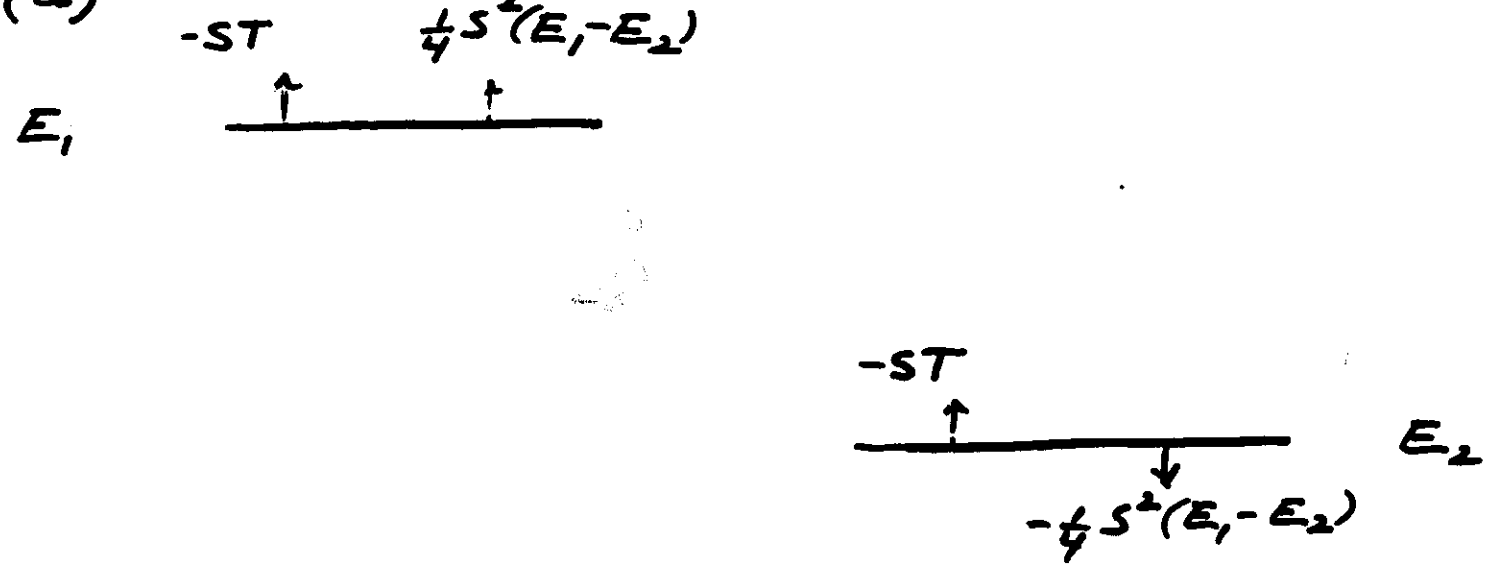
Metal - He interaction

PRB 39, 5684 (89)



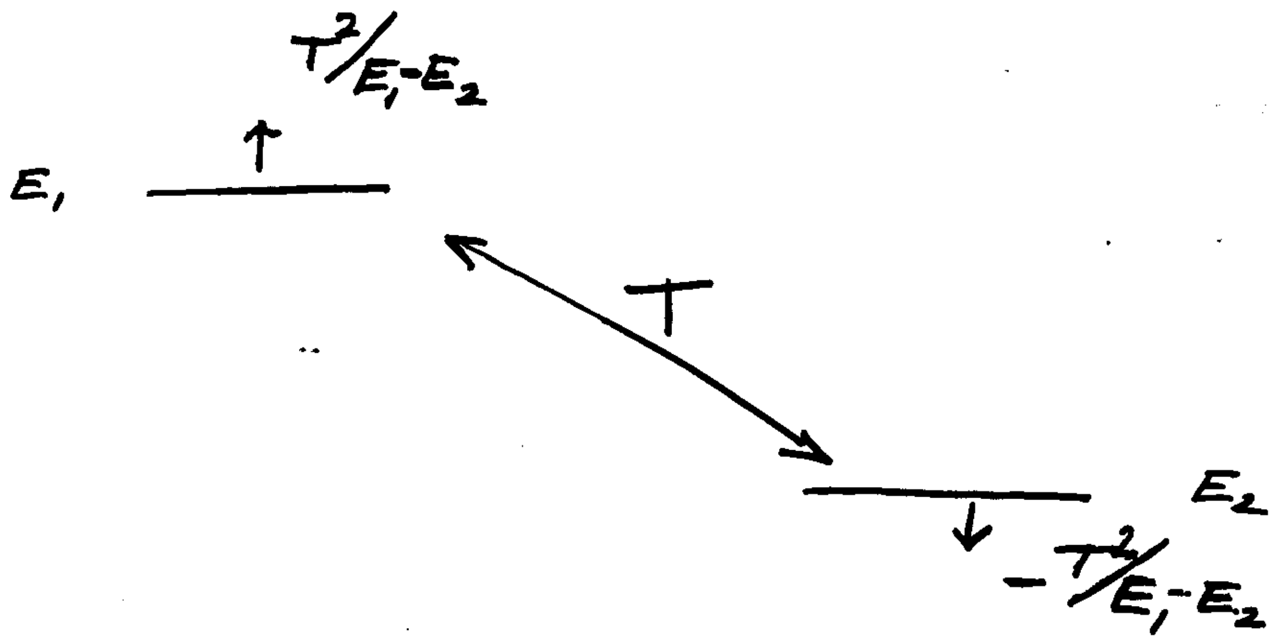
One-electron interaction

(a)



repulsive kinetic energy

(b)



$$(a) + (b) \qquad + \qquad T = -\tfrac{1}{2} S (E_1 - E_2)$$

$$\delta E_1 = S^2 (E_1 - E_2)$$

$$\delta E_2 = 0$$

$$V_{repulsive} = S^2(E_1 - E_2) + \tilde{J}_x + V_{electrostatic}$$

$$\tilde{J}_x = -\alpha \; S^2$$

$$V_{electrostatic} = -\beta \, S^2$$

$$V_{repulsive} = S^2 \Big\{ \underbrace{(E_1 - E_2)}_{\text{one-electron term}} - \underbrace{(\alpha + \beta)}_{\text{many-body interaction}} \Big\}$$

$$S^2 \sim n_M(\mathrm{He})$$ (metal density at the He-site)

$$V_{repulsive}\,(\text{He-metal}) = \gamma \; n_M(\mathrm{He})$$

$$\gamma \simeq 500 \ \mathrm{eV}\, a_0^3$$

$$\hat{H} = \hat{H}^{(0)}_{metal} + \hat{H}^{(0)}_{He} + \hat{V}_{interact.}$$

In our LCAO method:

$$(\hat{V}_{int.})_{i i'} = S_{i,He}\, S_{He,i'} \left\{ (E_M - E_{He}) - (\alpha + \beta) \right\} \equiv$$

$$\equiv V_0\, S_{i,He}\, S_{He,i'}$$

Compare with

$$V_{repulsive} = S_{i,He}^2 \left\{ (E_M - E_{He}) - (\alpha + \beta) \right\} \equiv V_0\, S_{i,He}^2$$

$$S_{i,He} = \int \psi_i\, \psi_{He}\, d^3r$$

$S_{i,He}$ is time-dependent through ψ_{He}

We assume to know the metal eigen-functions and eigenvalues:

$$\hat{H}^0 |n\rangle = E_n |n\rangle$$

Then:

$$S = \frac{1}{V}\frac{dE}{dx} = \frac{2}{V^2} \mathrm{Re} \sum_n \int_{-\infty}^{t} dt' \frac{e^{-i\omega_{n0}(t-t')}}{\hbar\omega_{n0}}$$

$$\langle 0| \frac{d\hat{V}_{int}(t)}{dt} |n\rangle \langle n| \frac{d\hat{V}_{int}(t')}{dt'} |0\rangle$$

In the simplest approximation:

$$|n\rangle \equiv |\vec{k}\rangle \equiv \frac{1}{S(k)} \sum_i e^{i\vec{k}\cdot\vec{R}_i} \varphi(\vec{r}-\vec{R}_i)$$

and

$$E_n \equiv \varepsilon(k) \qquad\qquad S(k) = \sum_R e^{i\vec{k}\cdot\vec{R}} S(\vec{R})$$

$$\frac{1}{v}\frac{dE}{dx} = 2\pi V_0^2 \int_{-\infty}^{\infty} \frac{d^3q}{(2\pi)^3}\frac{d^3k}{(2\pi)^3}\frac{\bar{q}\cdot\bar{v}}{v^2}\,\theta(k_F-k)\,\theta(k'-k_F)$$

$$\sum_{G} e^{-i\bar{G}\cdot\bar{R}}\,\frac{1}{S(k)}\Big\{\sum_{R_1} e^{i(\bar{k}-\bar{q})\cdot\bar{R}_1}\,\Phi^{R_1}(\bar{q})\Big\}\times$$

$$\times\,\frac{1}{S(k')}\Big\{\sum_{R_2} e^{-i(\bar{k}-\bar{q}-\bar{G})\cdot\bar{R}_2}\,\Phi^{R_2}(\bar{q}+\bar{G})\Big\}\times$$

$$\times\,\delta(\omega_{kk'}+\bar{q}\cdot\bar{v}+\bar{G}\cdot\bar{v})$$

$$\Phi^{R_2}(q) = \int \psi(\bar{r}-\bar{R}_2)\,\psi(\bar{r})\,e^{i\bar{q}\cdot\bar{r}}\,d\bar{r}$$

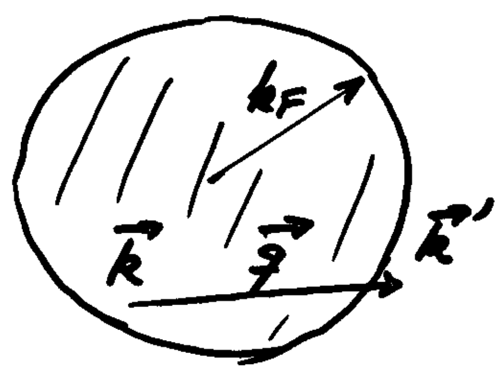
$G = 0$

Then :

$$\frac{1}{V}\frac{dE}{dx} = -\pi V_0^2 \int_{-\infty}^{\infty} \frac{d^3q}{(2\pi)^3}\,\frac{d^3k}{(2\pi)^3}\,\frac{\vec{q}\cdot\vec{v}}{v^2}\,\theta(k_F-k)\,\theta(k'-k_F)$$

$$\times\frac{1}{S(k)}\left\{\sum_{R_1} e^{i(\vec{k}-\vec{q})\cdot\vec{R}_1}\,\Phi^{R_1}(q)\right\}\frac{1}{S(k')}\left\{\sum_{R_2} e^{-i\vec{k}'\cdot\vec{R}_2}\,\Phi^{R_2}(q)\right\}$$

$$\times\ \delta(\omega_{kk'}+\vec{q}\cdot\vec{v})$$



$$\Phi^{R}(\vec{q}) = \int \psi(\vec{r}-\vec{R})\,\psi(\vec{r})\,e^{i\vec{q}\cdot\vec{r}}\,d\vec{r}$$

Comparison with LDA

	Li	Na	K	Rb
ENR	0.10	0.053	0.023	0.016
LCAO	0.26	0.086	0.023	0.014

$\frac{1}{v}\frac{dE}{dx}$ (a.u.)

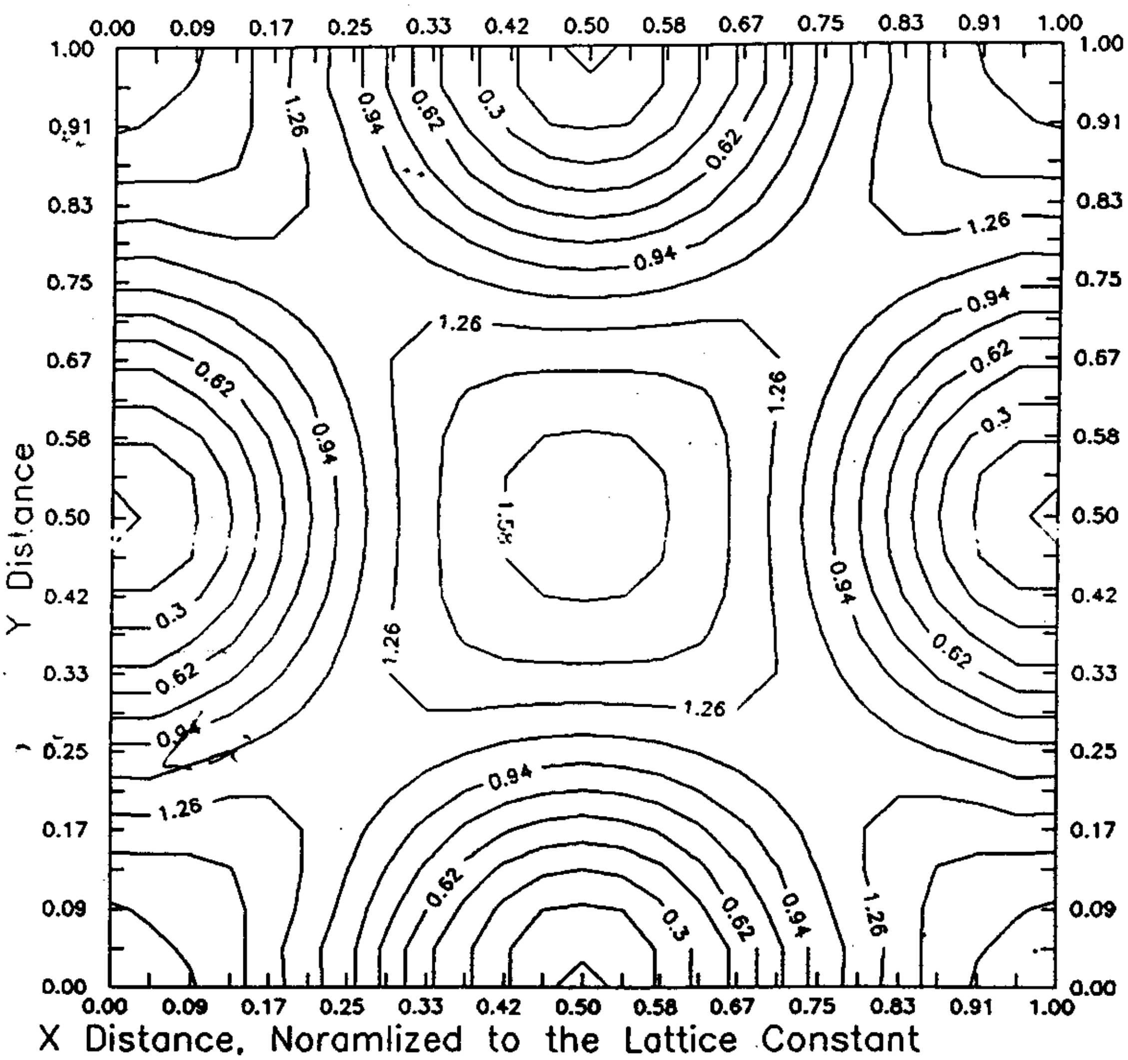
For Li and Na, the p-band is important, explaining the discrepancy with ENR. For K and Rb (s-like bands) the agreement is excellent

In Li $r_s \simeq 0.52$

In Rb and K [illegible] $r_s \simeq 0.80$

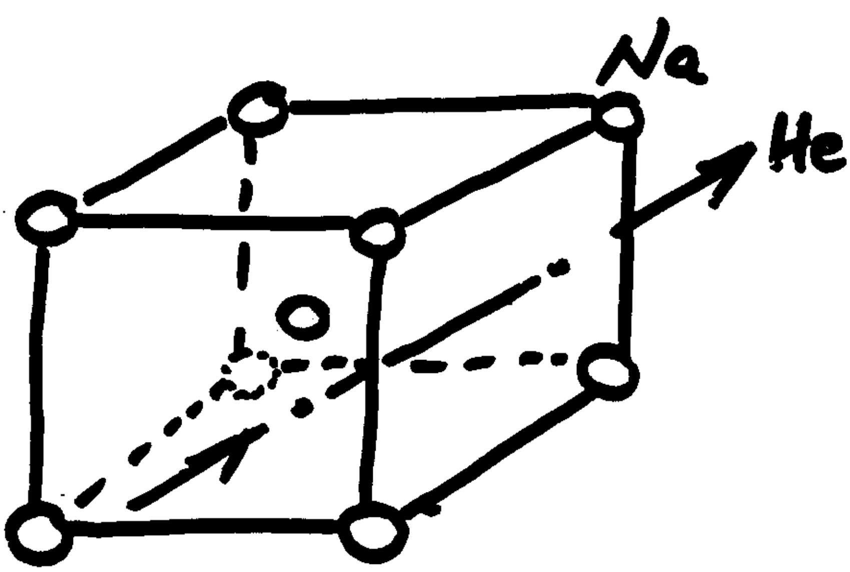
He/Na

Fig 3.

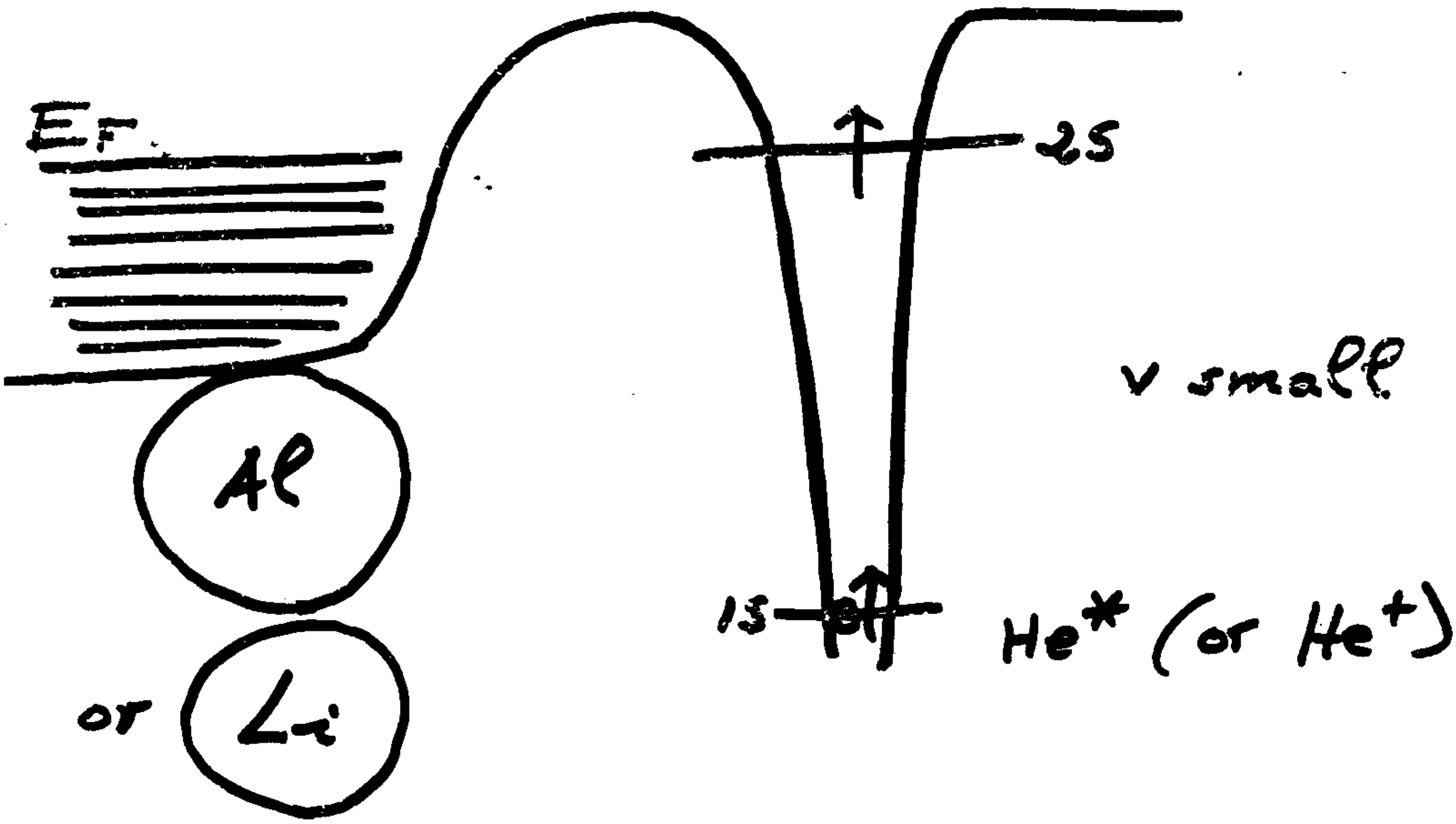


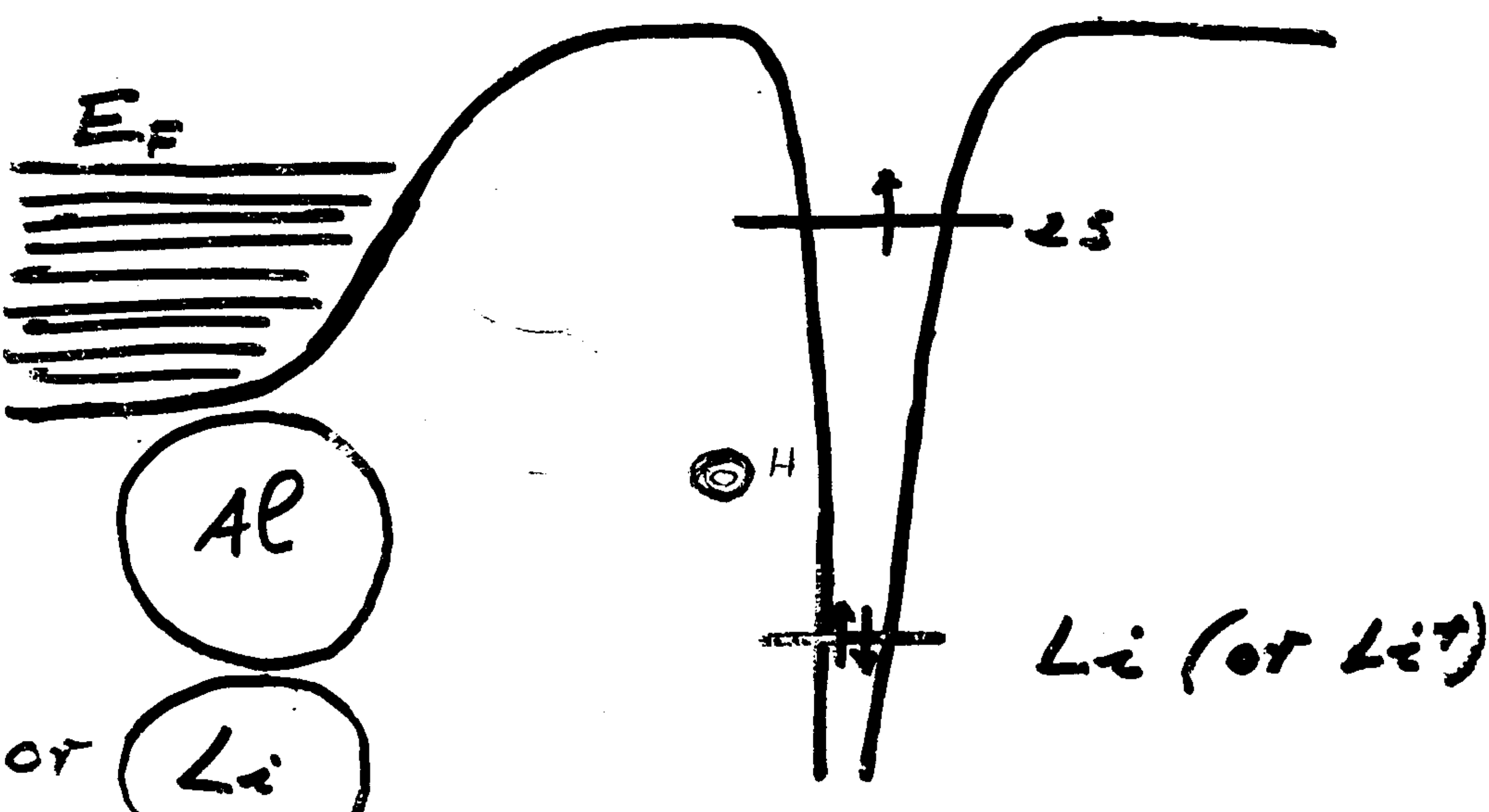
S/S_0

$S_0 \equiv$ mean stopping power

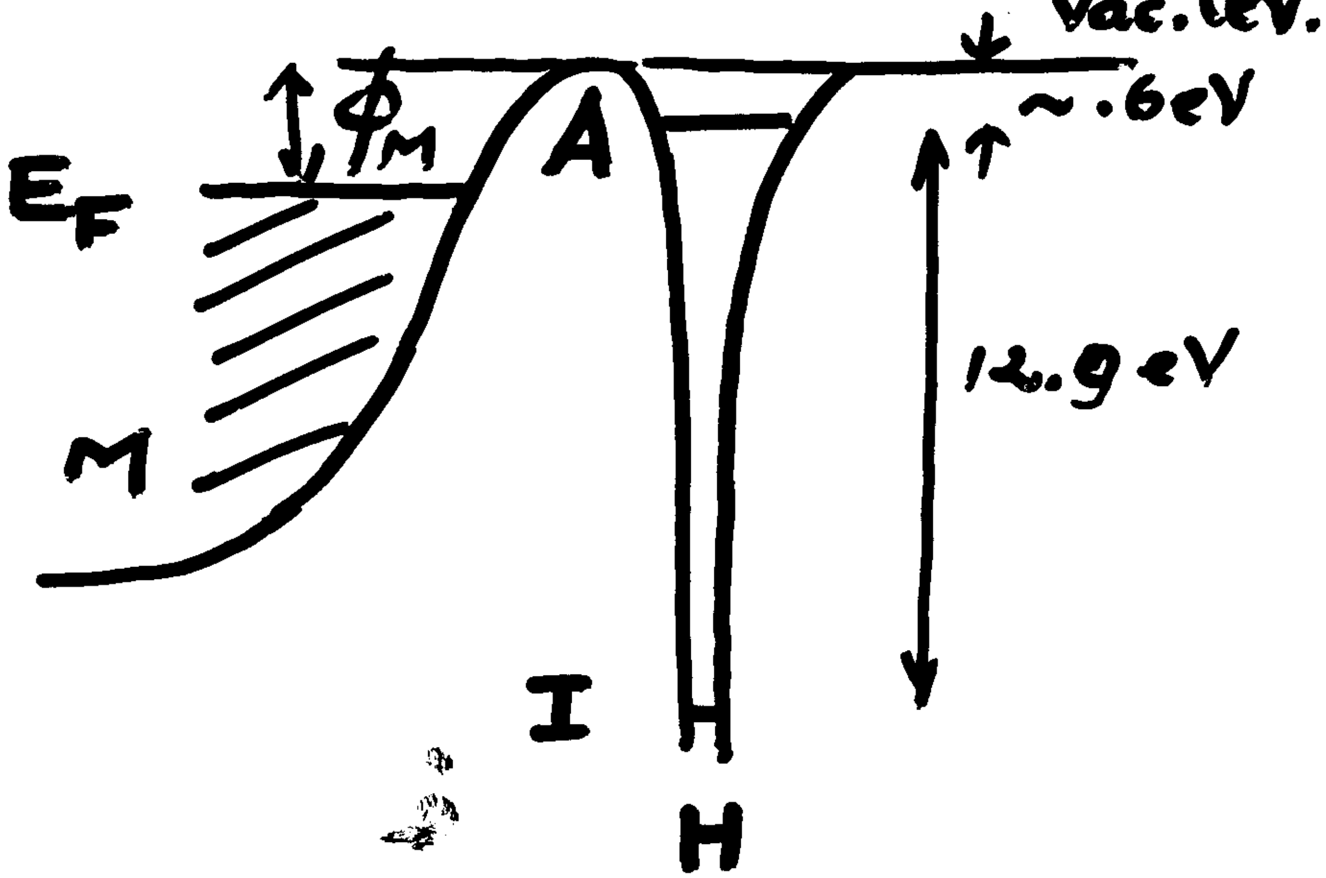


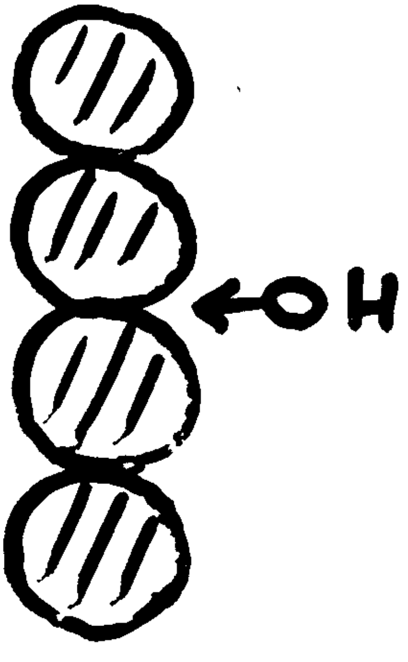
Charge transfer processes





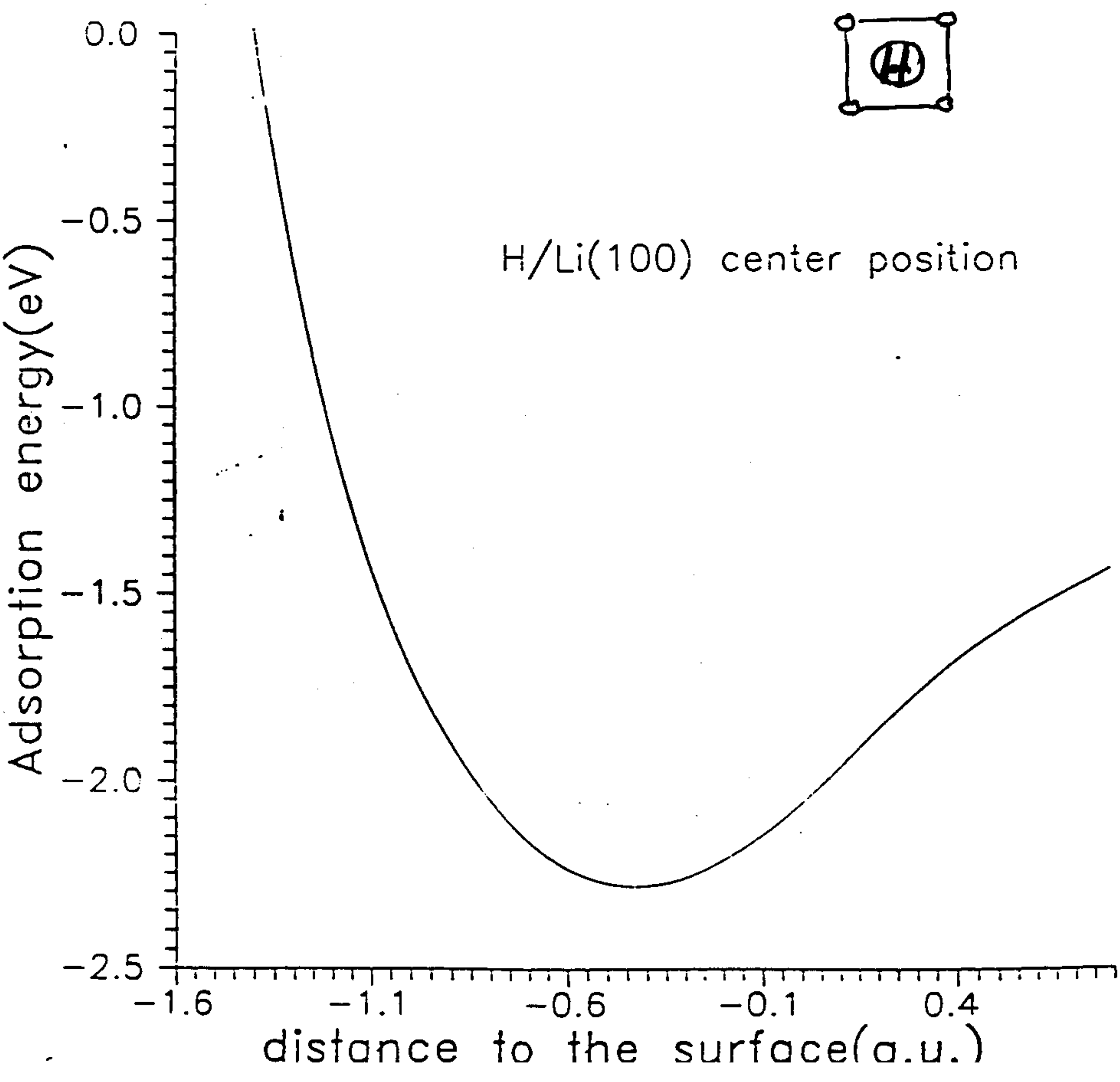
H-Metal interaction



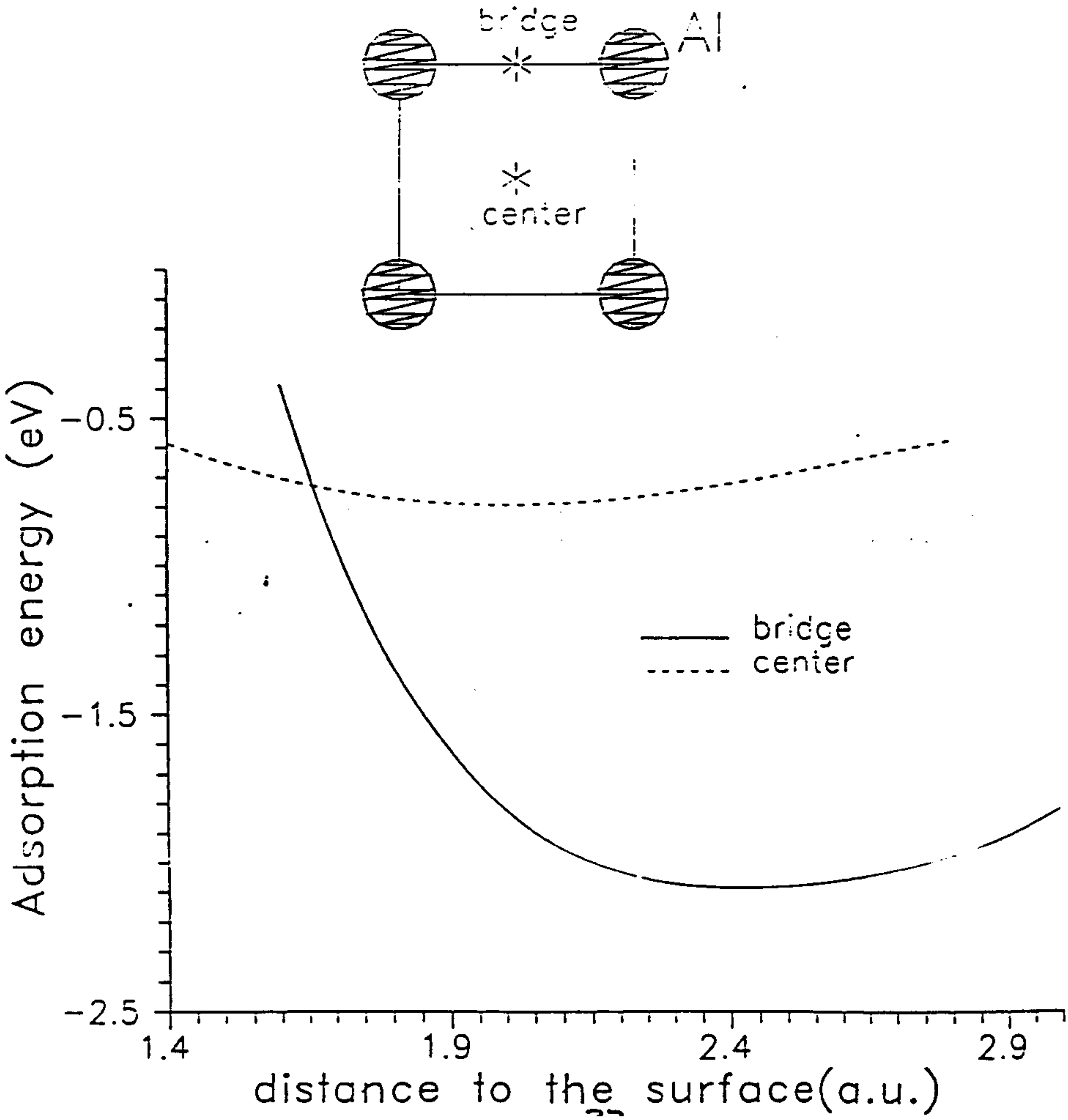


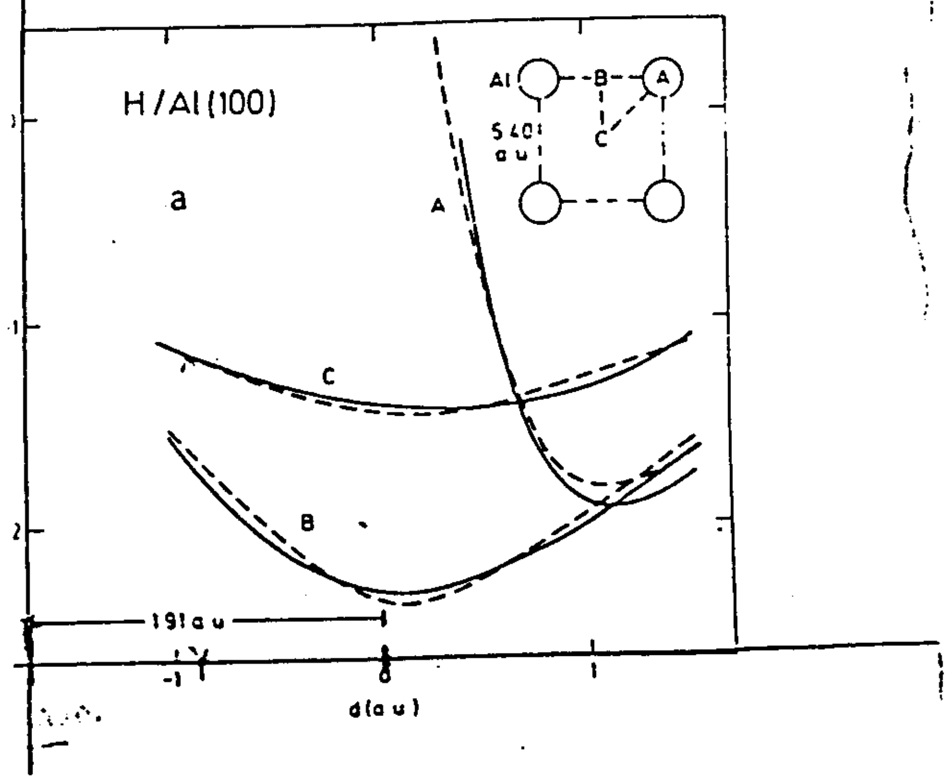
PRB (91)

GARCIA-VIDAL ET AL. FIGURE 9



GARCIA-VIDAL ET AL. FIGURE 5




H / Al(100)
a
A
B
C
Al
5.40 a.u.
1.91 a.u.
-1
0
1
2
d(a.u.)

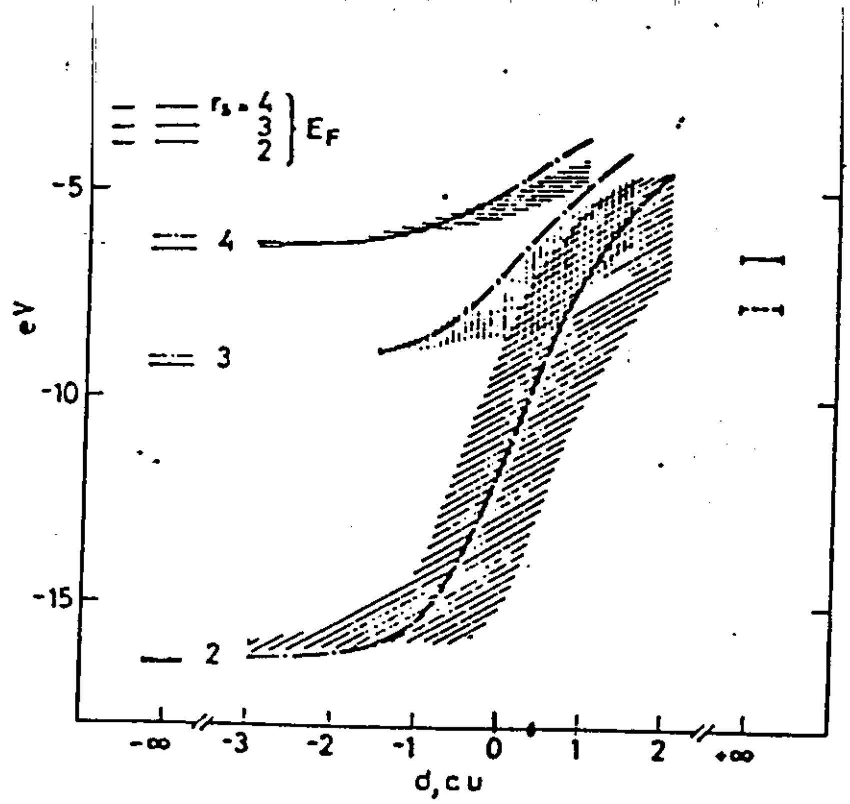


Fig. 4. The peak position (shaded area) in the H-induced density of states [4], as a function of the distance d between the H atom and the jellium edge is shown for the different r_s values. The dash-dotted curves gives the effective electron potential of the clean surface, $V_{eff}^0(d)$. To the left ($d = -\infty$), the bulk results [16] are given. To the right ($d = \infty$), the free-atom results are given both for a spin-polarized (dashed line) and an unpolarized (full line) calculation.

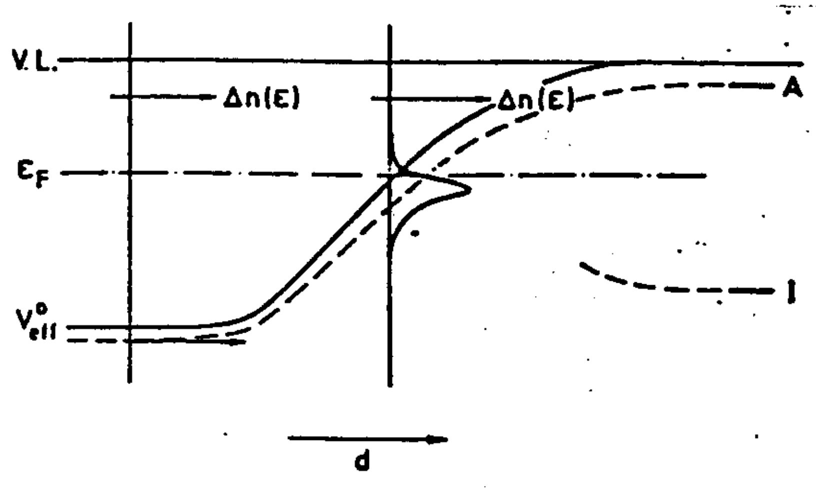
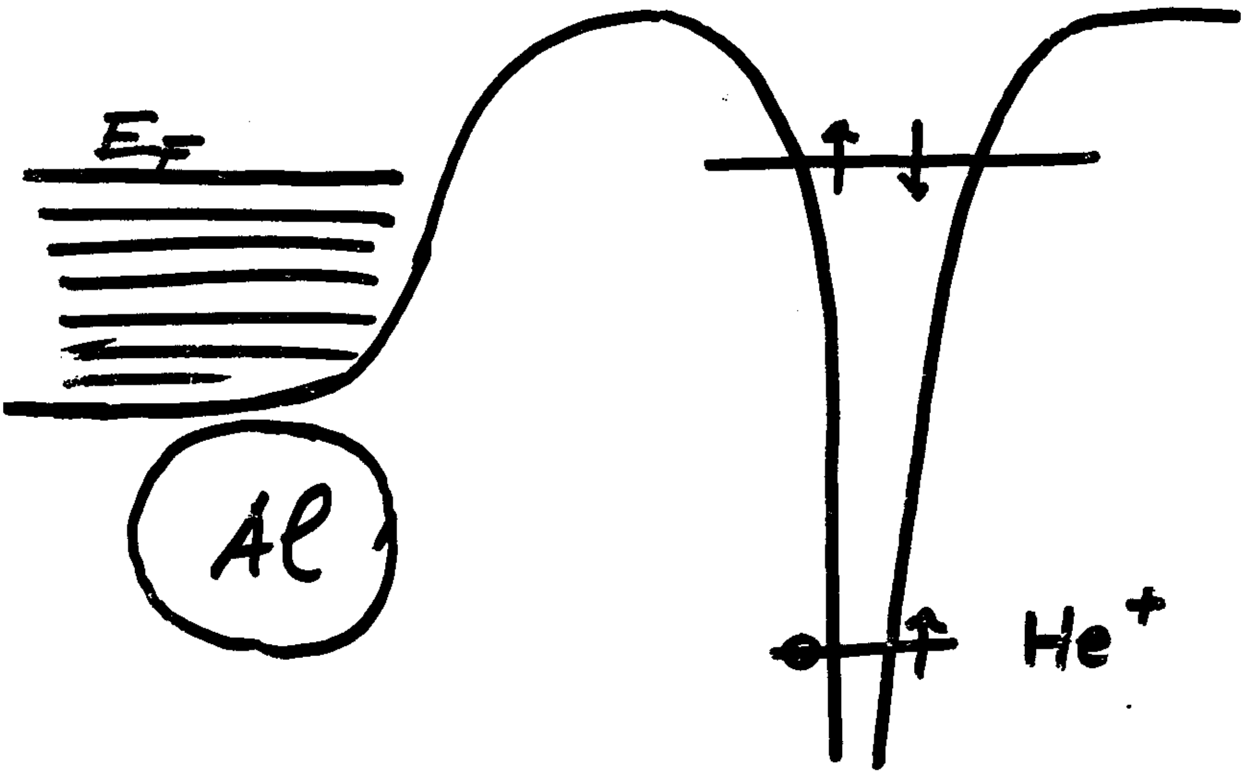
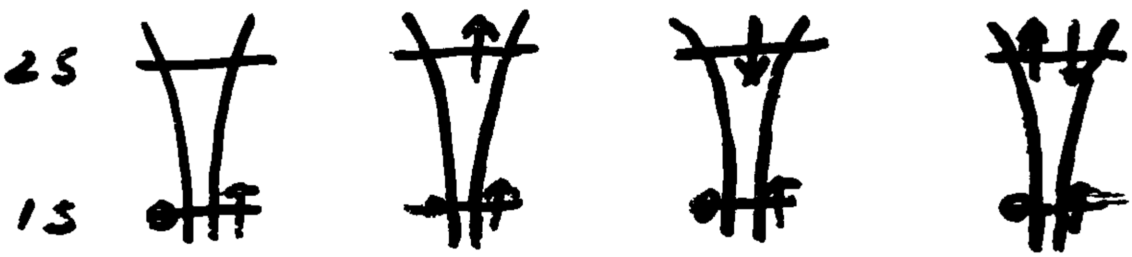


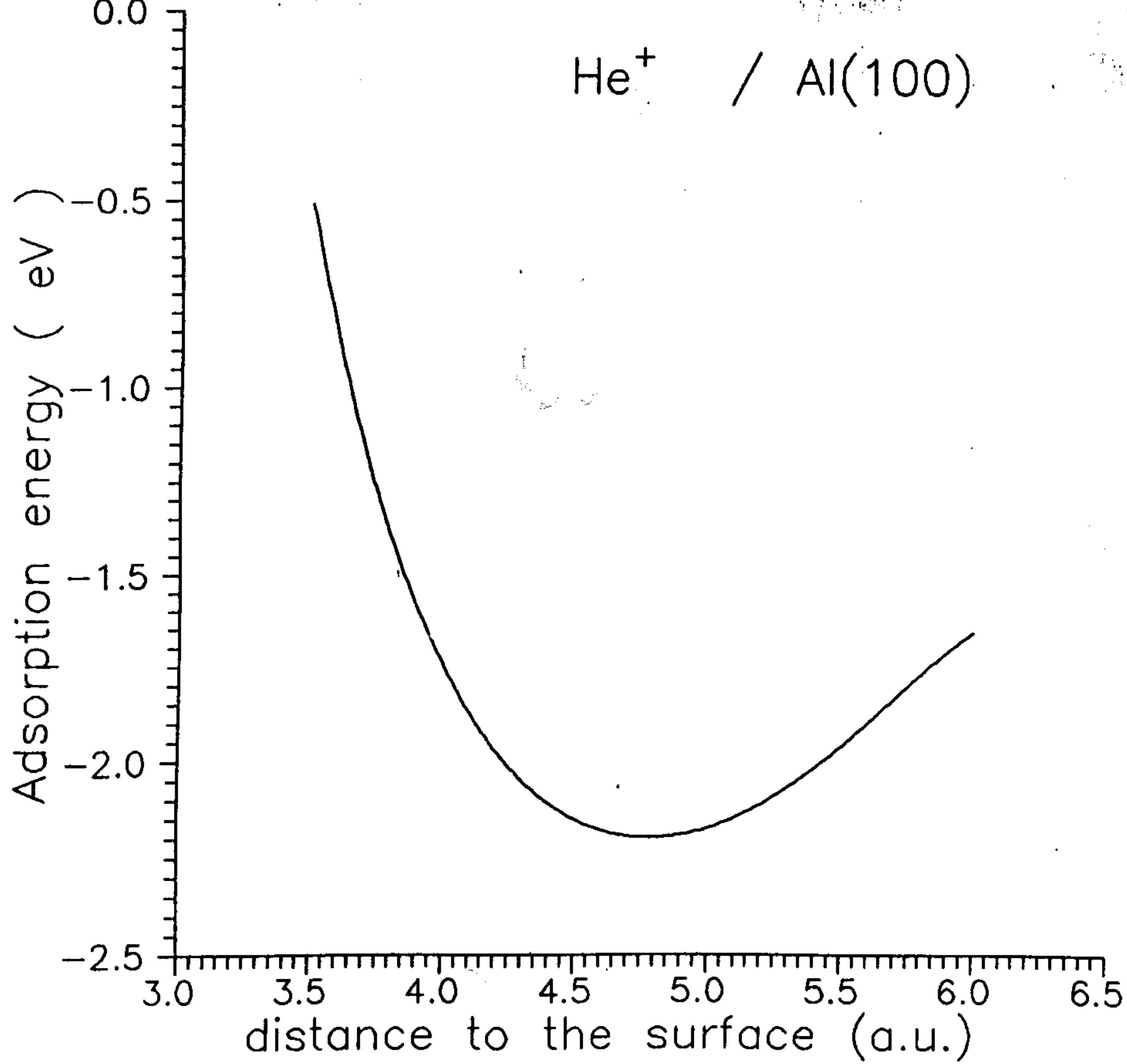
Fig. 6. Schematic drawing of the hydrogen-induced one-electron spectrum for the H–Je system in its ground state, for varying distances d between the proton and the jellium edge. The vacuum level (V.L.), the work function ϕ, the Fermi level (ϵ_F) and the bottom of the conduction band ($V_{eff}^{\prime 0}$) of the substrate are marked, as well as the affinity (A) and ionization levels (I) of the free H atom. The dashed curve indicates the variation of the level for the non-adiabatic state, leading to the H^- ion upon rapid separation.

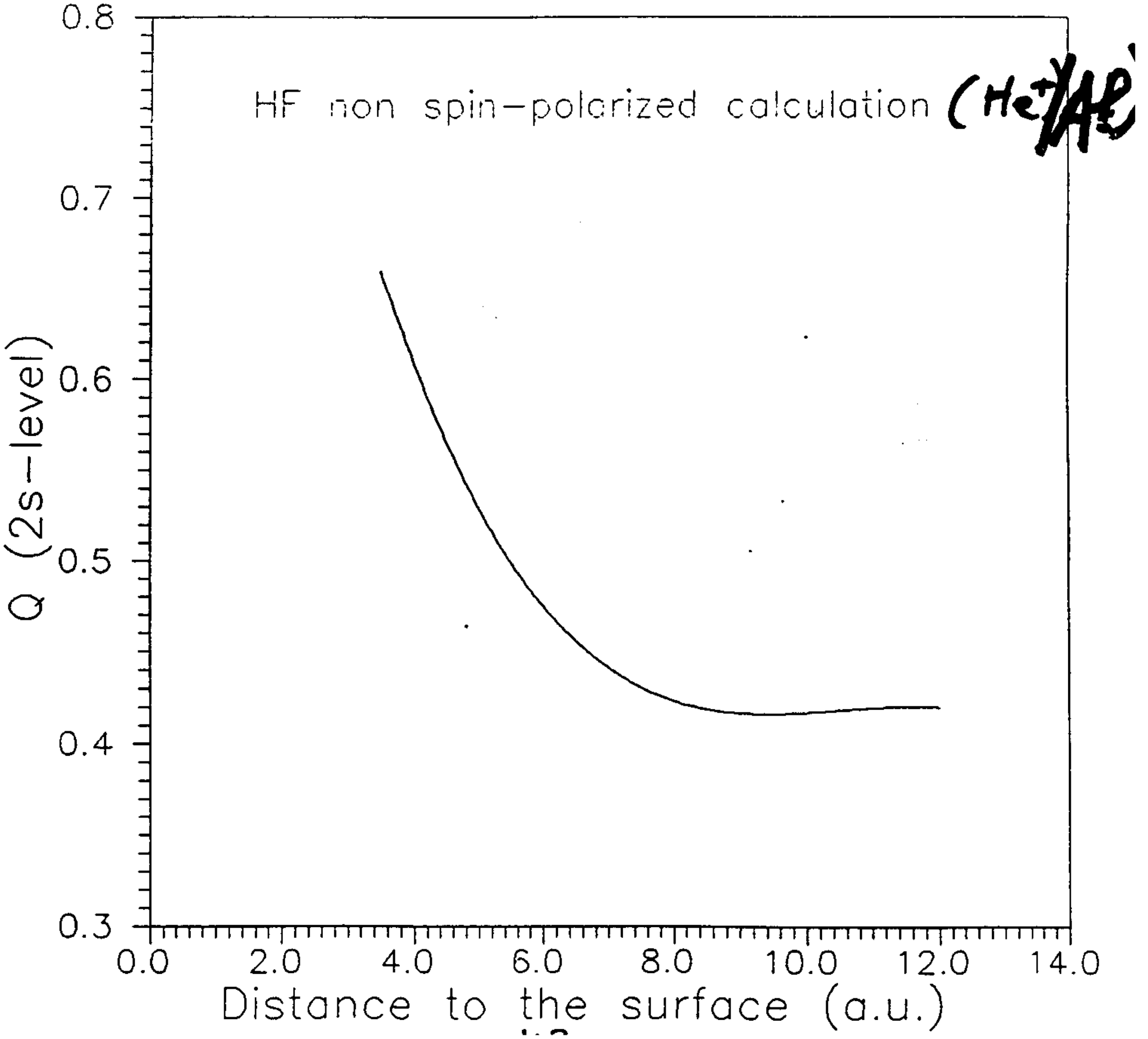
HF- calculation



He-states

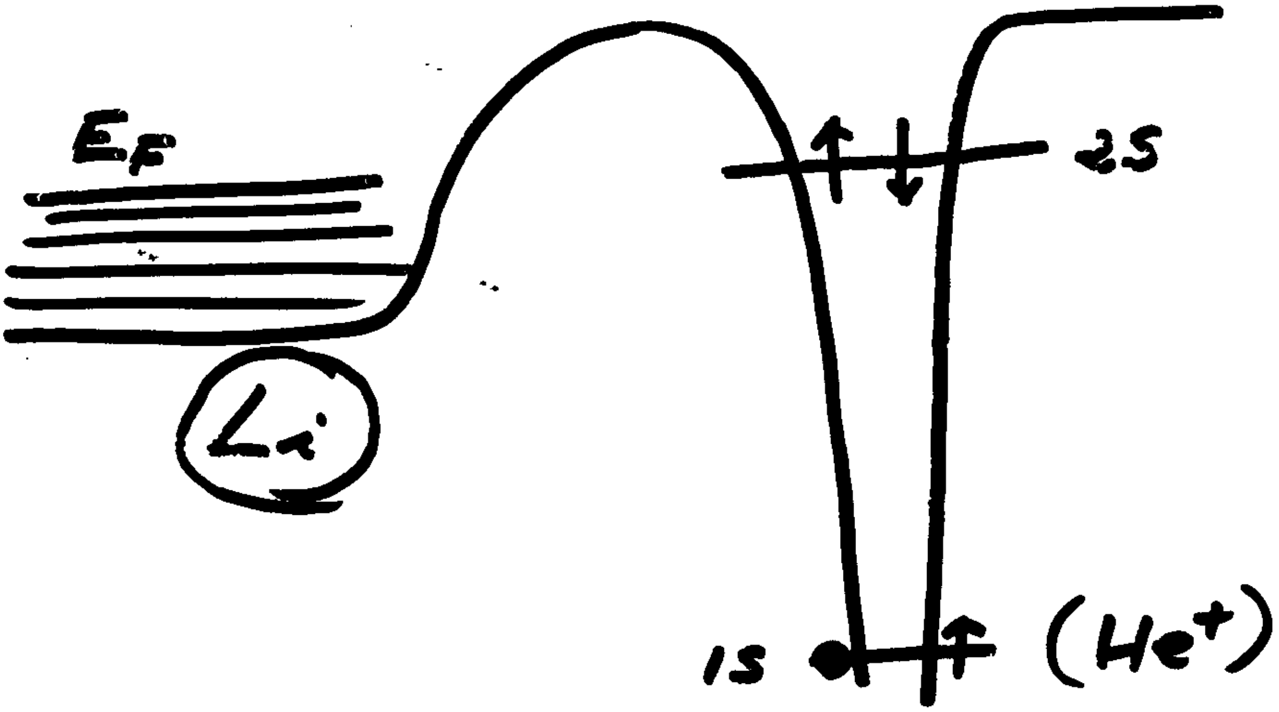



He+ / Al(100)
Adsorption energy (eV)
0.0
−0.5
−1.0
−1.5
−2.0
−2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
distance to the surface (a.u.)

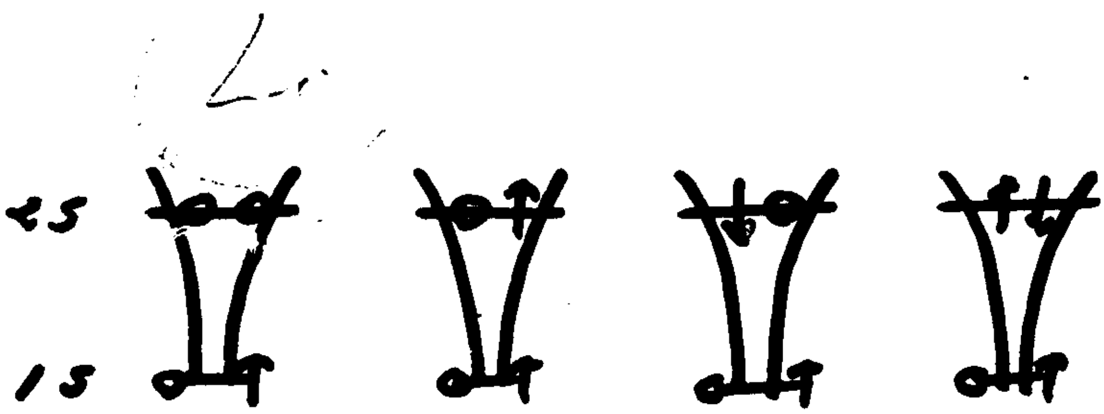


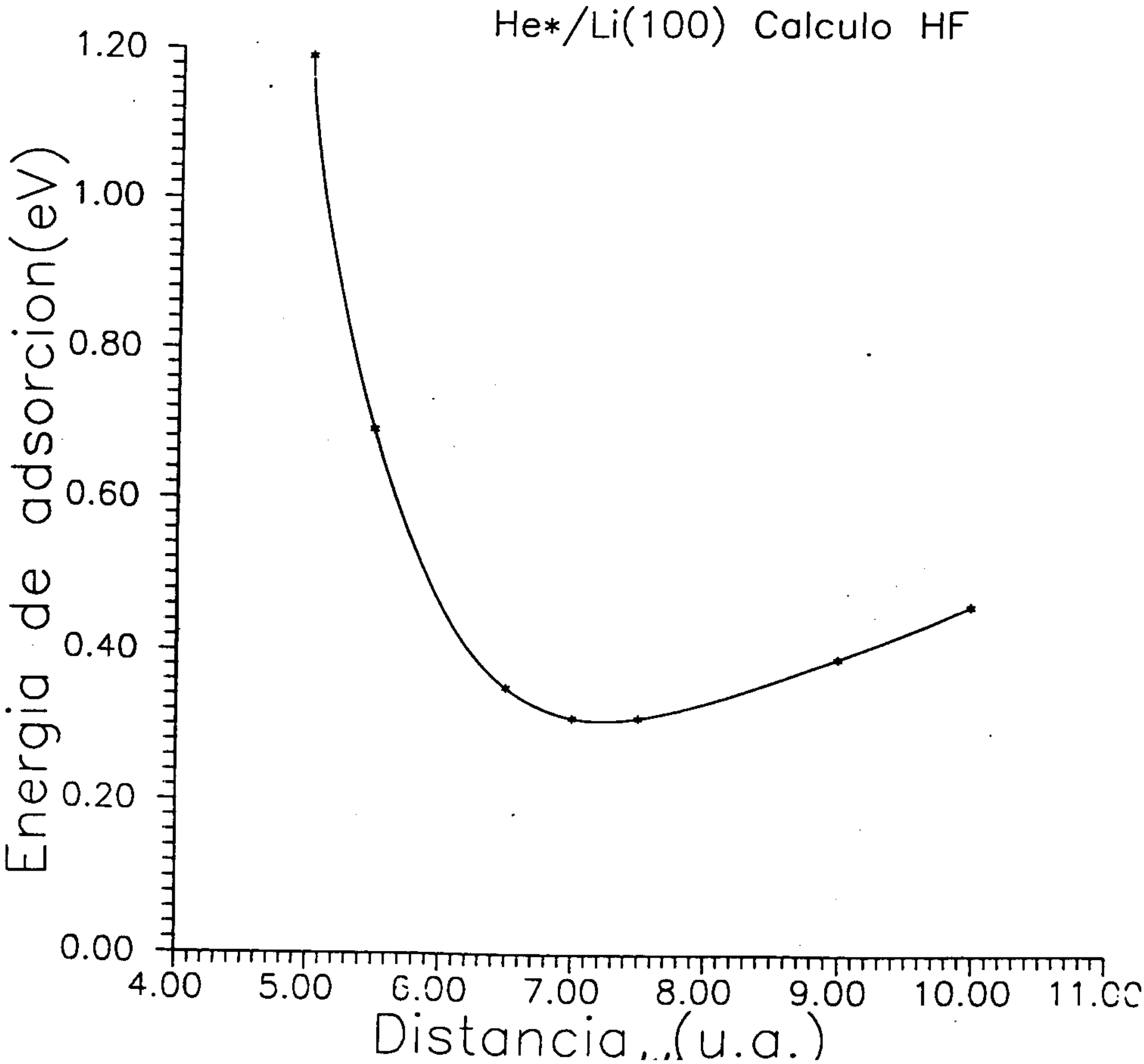
HF non spin-polarized calculation (He⁺/Al)
Q (2s-level)
Distance to the surface (a.u.)
0.3
0.4
0.5
0.6
0.7
0.8
0.0
2.0
4.0
6.0
8.0
10.0
12.0
14.0

HF-calculation

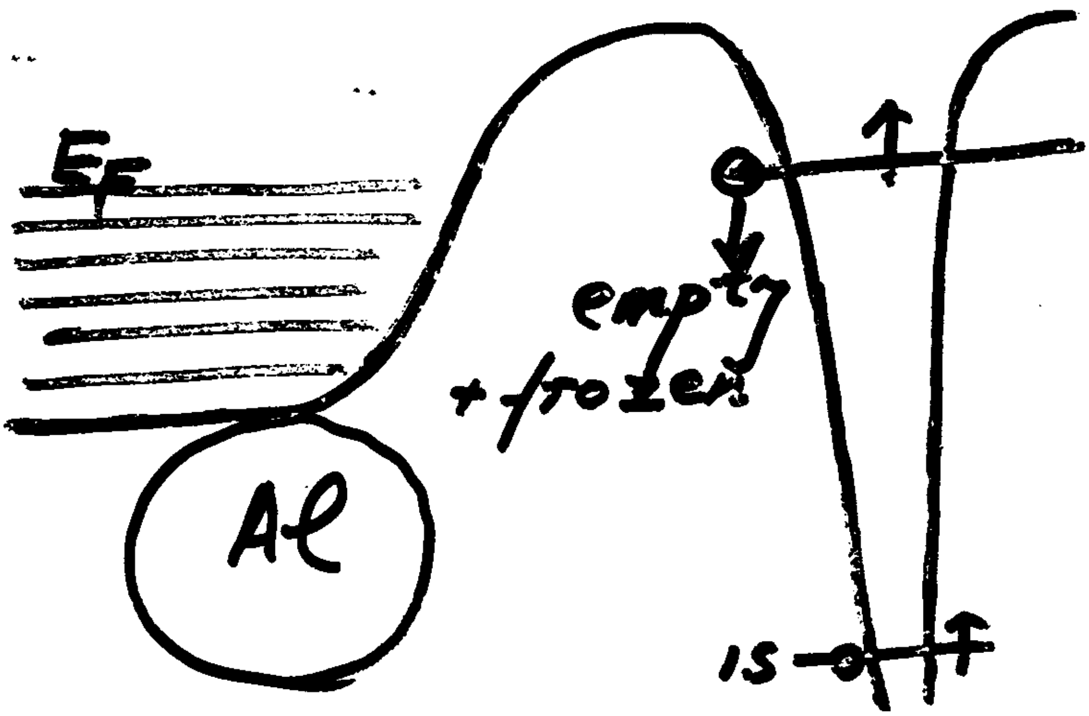


He-states

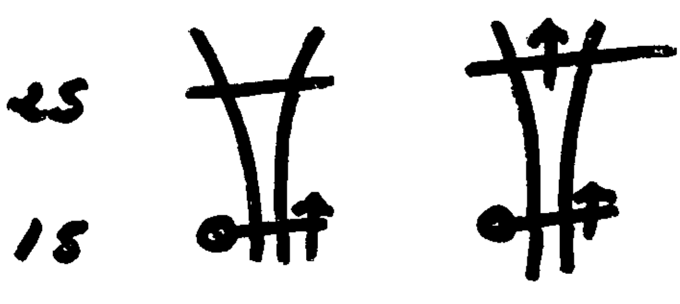



He*/Li(100) Calculo HF
Energia de adsorcion(eV)
0.00
0.20
0.40
0.60
0.80
1.00
1.20
4.00
5.00
6.00
7.00
8.00
9.00
10.00
11.00
Distancia (u.a.)

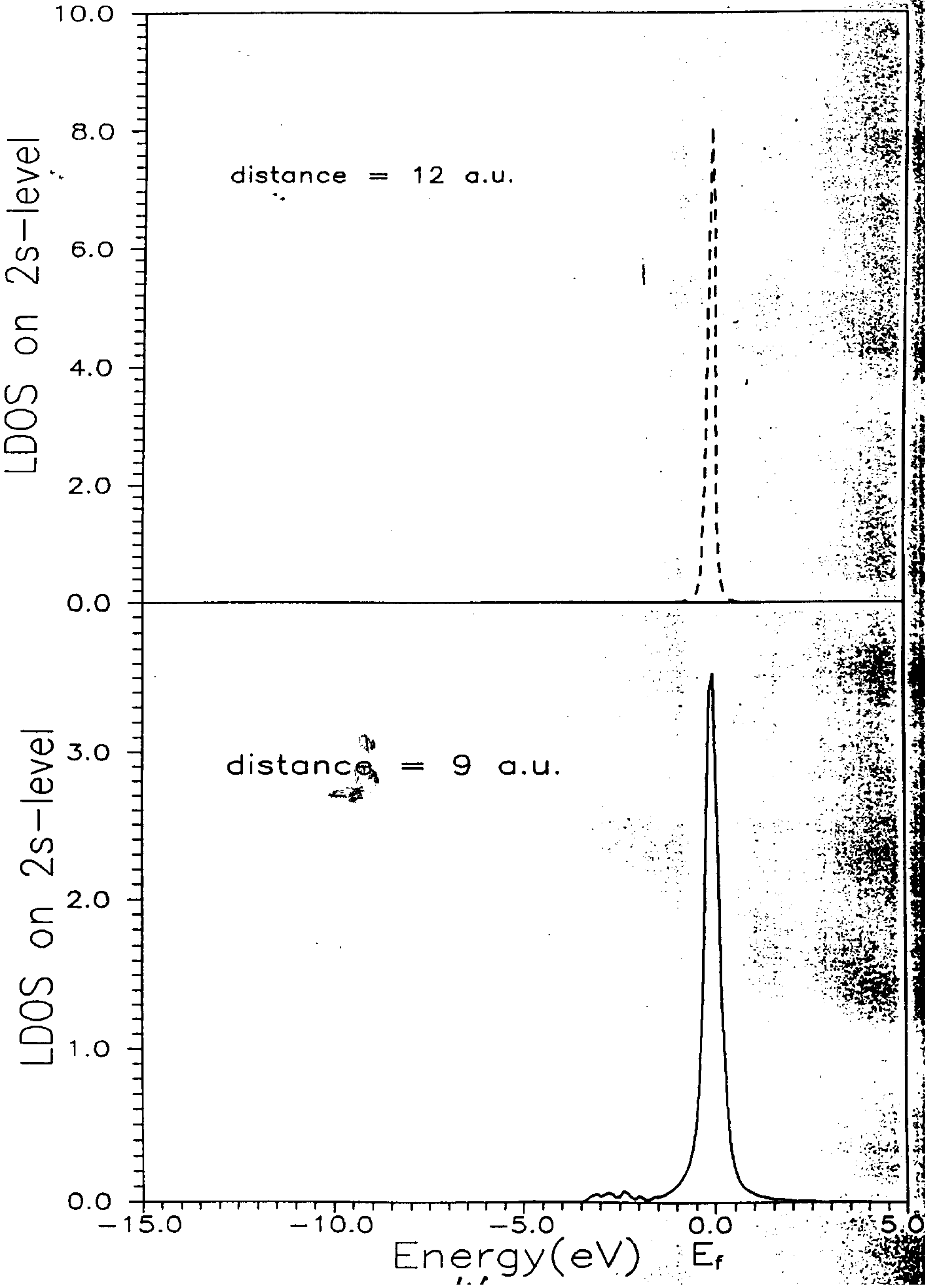
Spin-polarized calculation



He-states

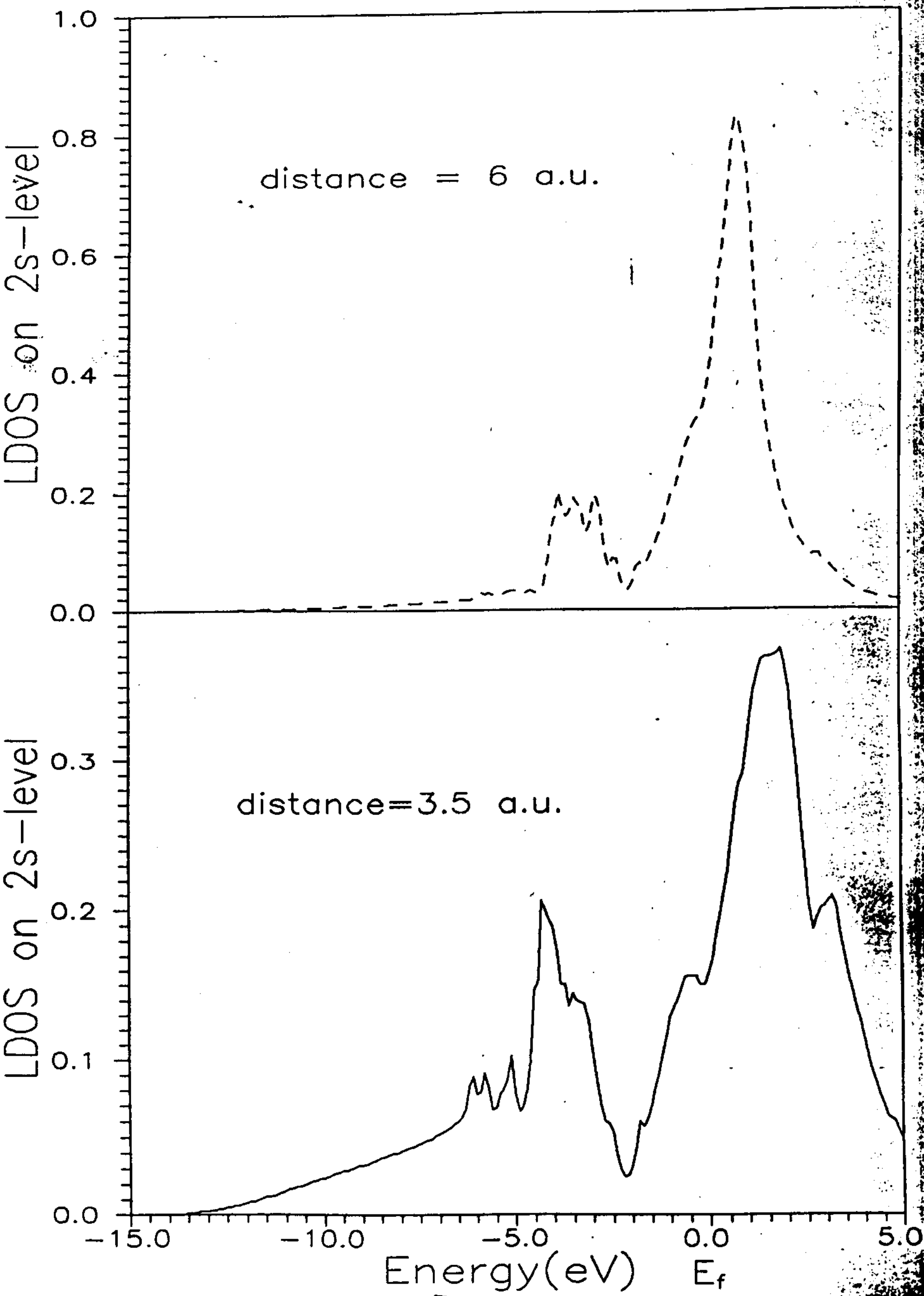


He*/Al

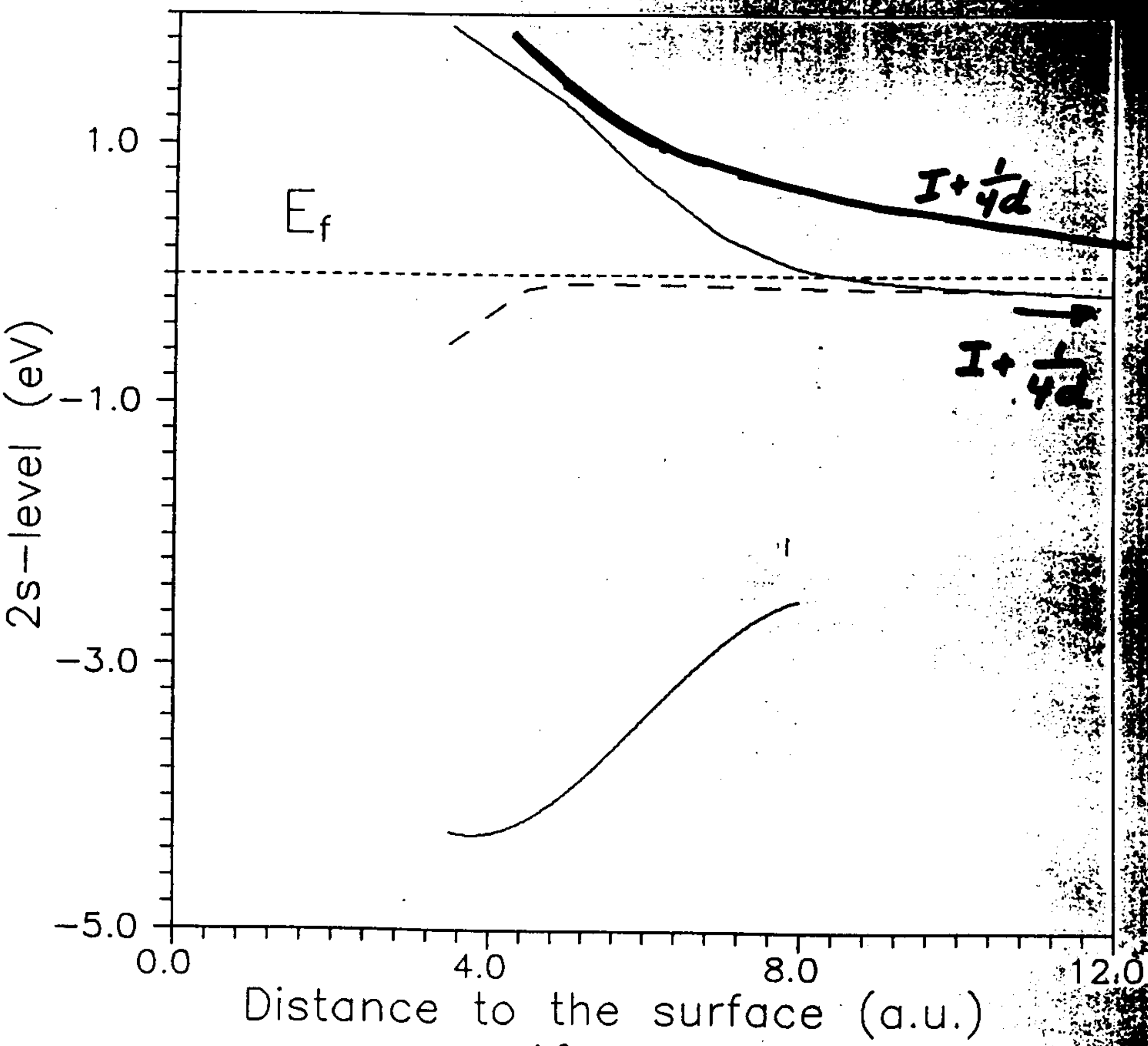


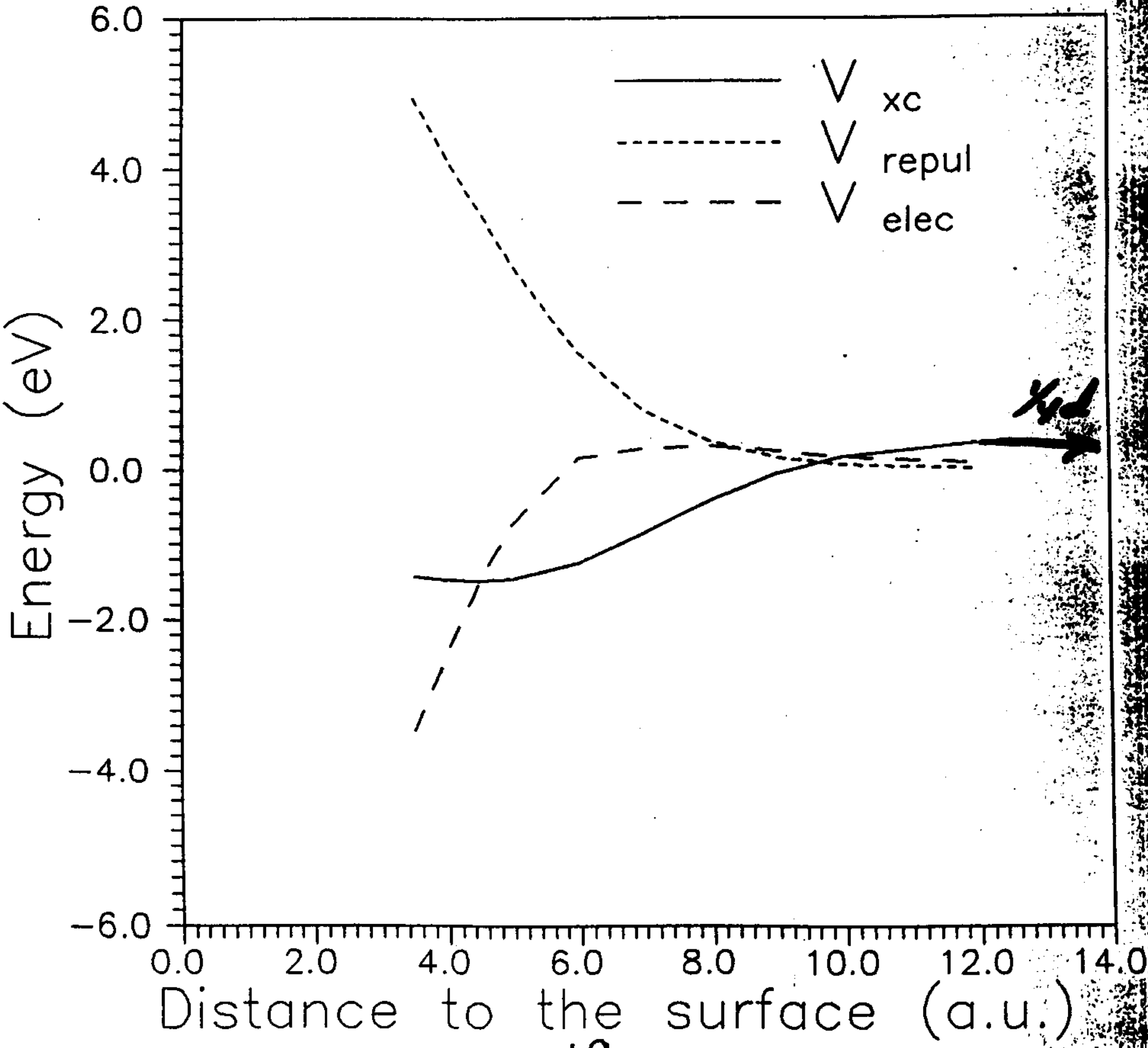
LDOS on 2s−level
distance = 12 a.u.
10.0
8.0
6.0
4.0
2.0
0.0
LDOS on 2s−level
distance = 9 a.u.
3.0
2.0
1.0
0.0
−15.0
−10.0
−5.0
0.0
5.0
Energy(eV)
E_f

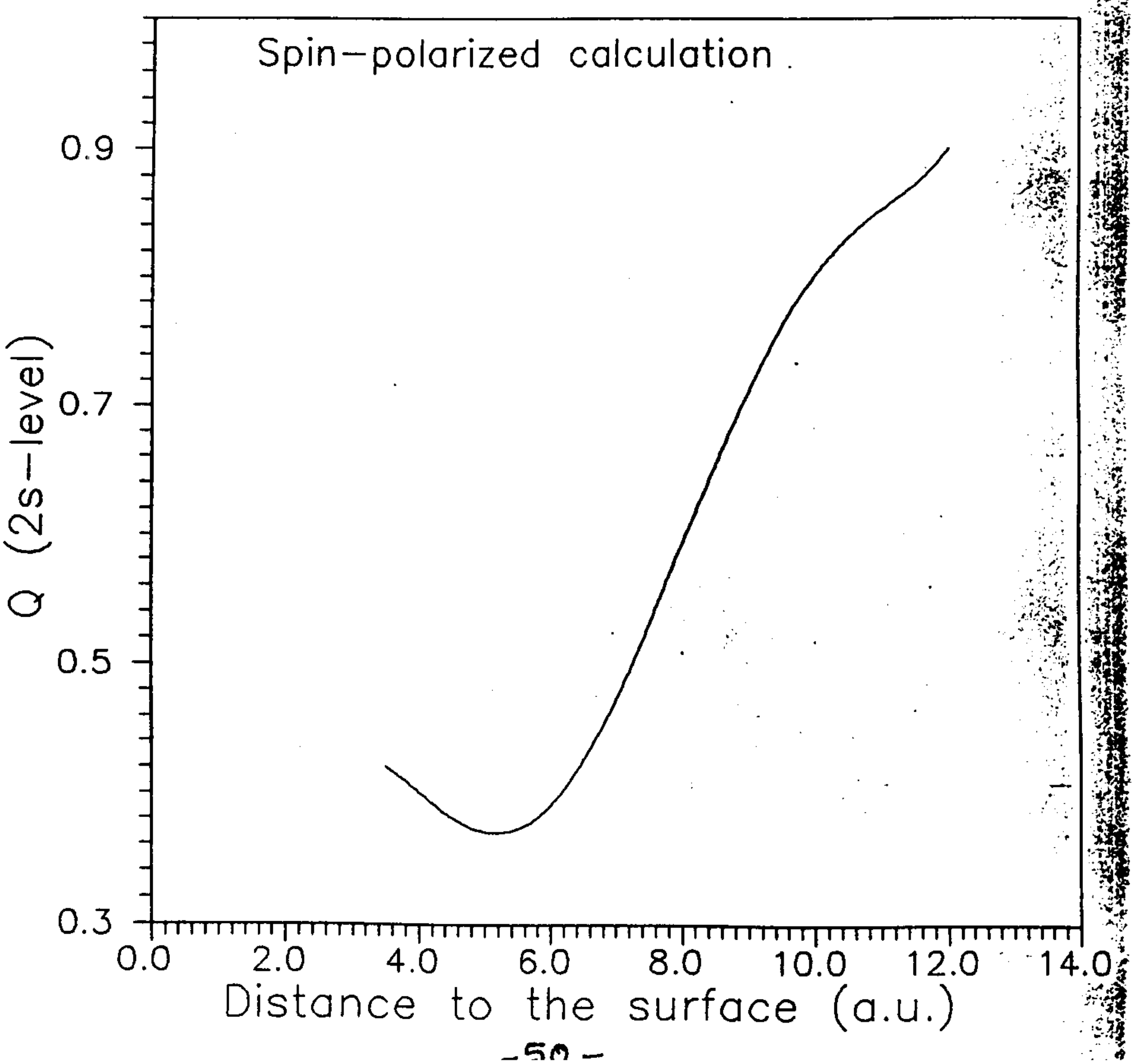
He/Al


LDOS on 2s-level
distance = 6 a.u.
LDOS on 2s-level
distance=3.5 a.u.
1.0
0.8
0.6
0.4
0.2
0.0
0.3
0.2
0.1
0.0
−15.0
−10.0
−5.0
0.0
5.0
Energy(eV)
E_f

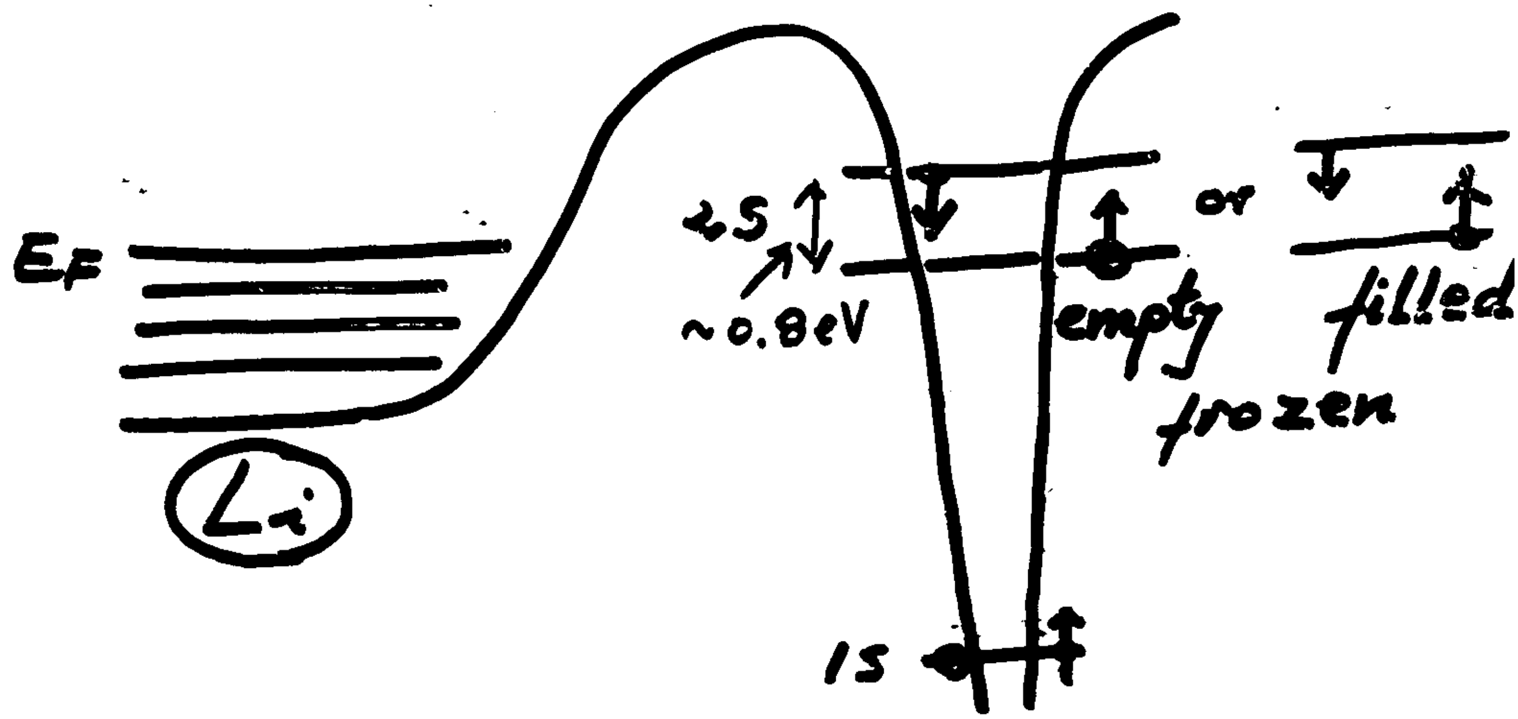
Spin-polarized calculation



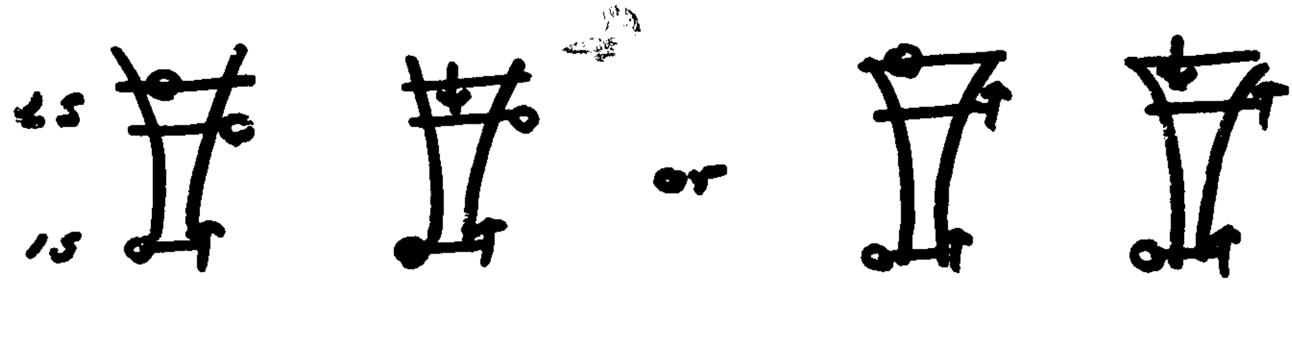

6.0
4.0
2.0
0.0
−2.0
−4.0
−6.0
Energy (eV)
V xc
V repul
V elec
¼d
0.0
2.0
4.0
6.0
8.0
10.0
12.0
14.0
Distance to the surface (a.u.)


Spin-polarized calculation
Q (2s-level)
0.3
0.5
0.7
0.9
0.0
2.0
4.0
6.0
8.0
10.0
12.0
14.0
Distance to the surface (a.u.)

Spin-polarized calculations

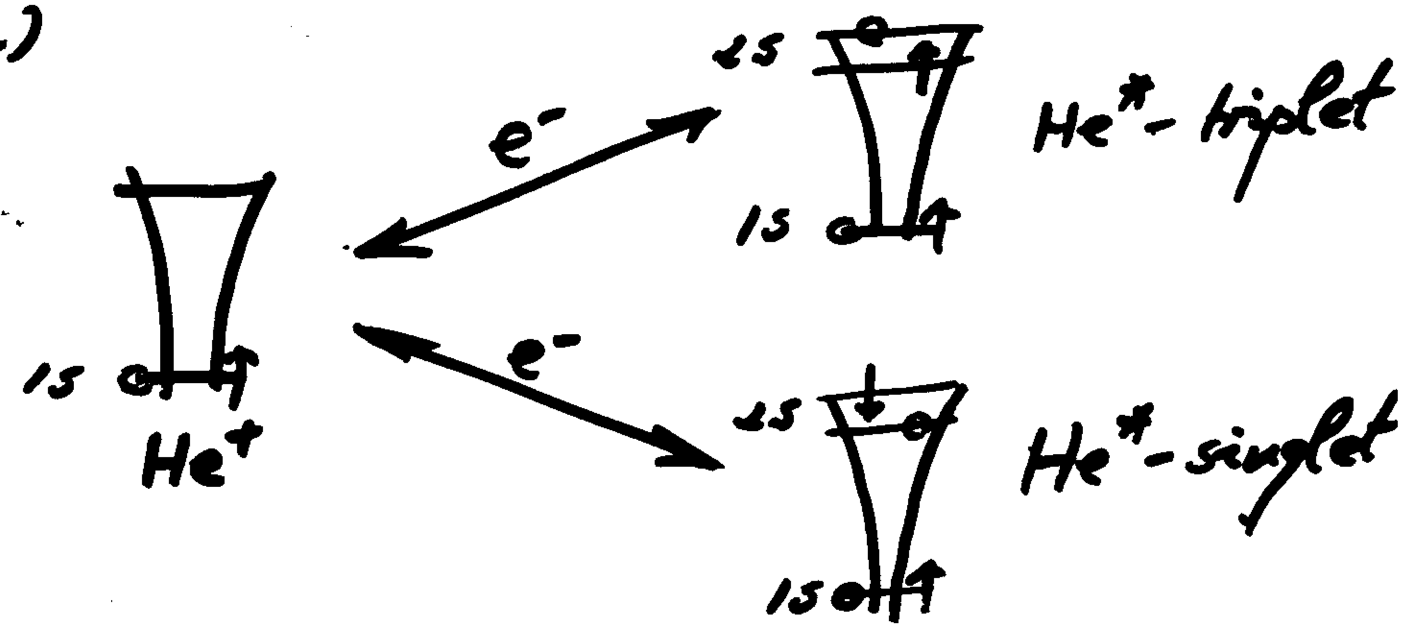


He-states

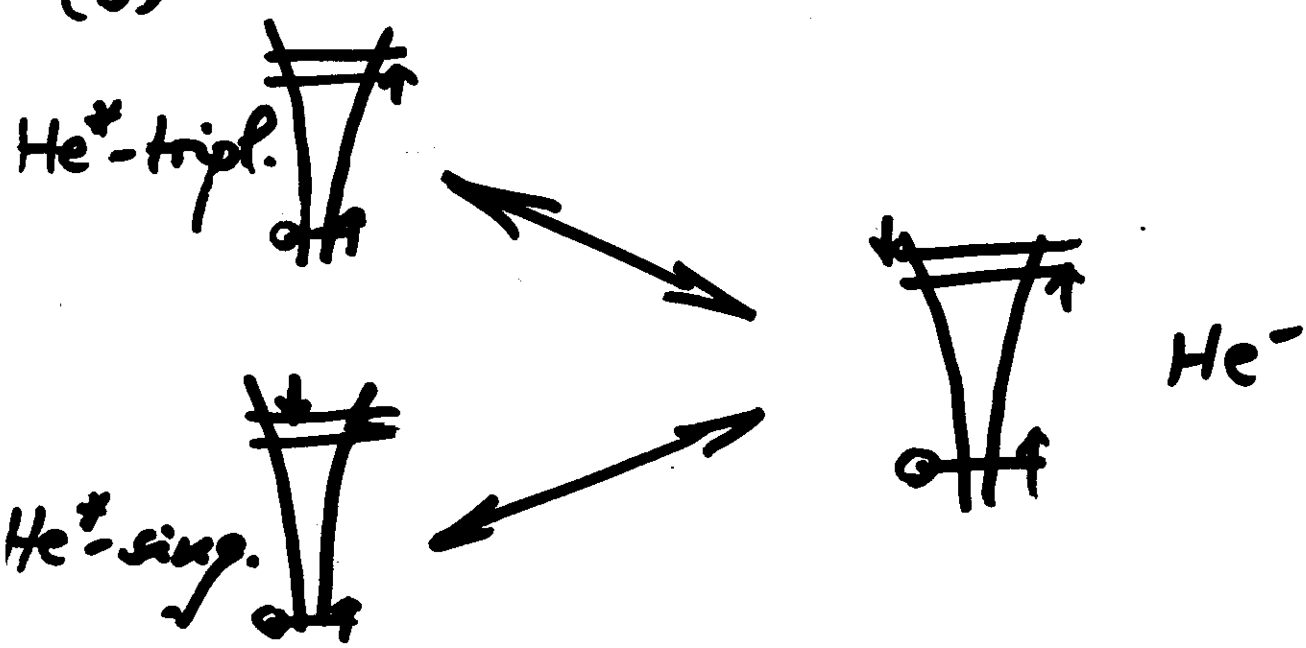


He^+ on Li

(a)

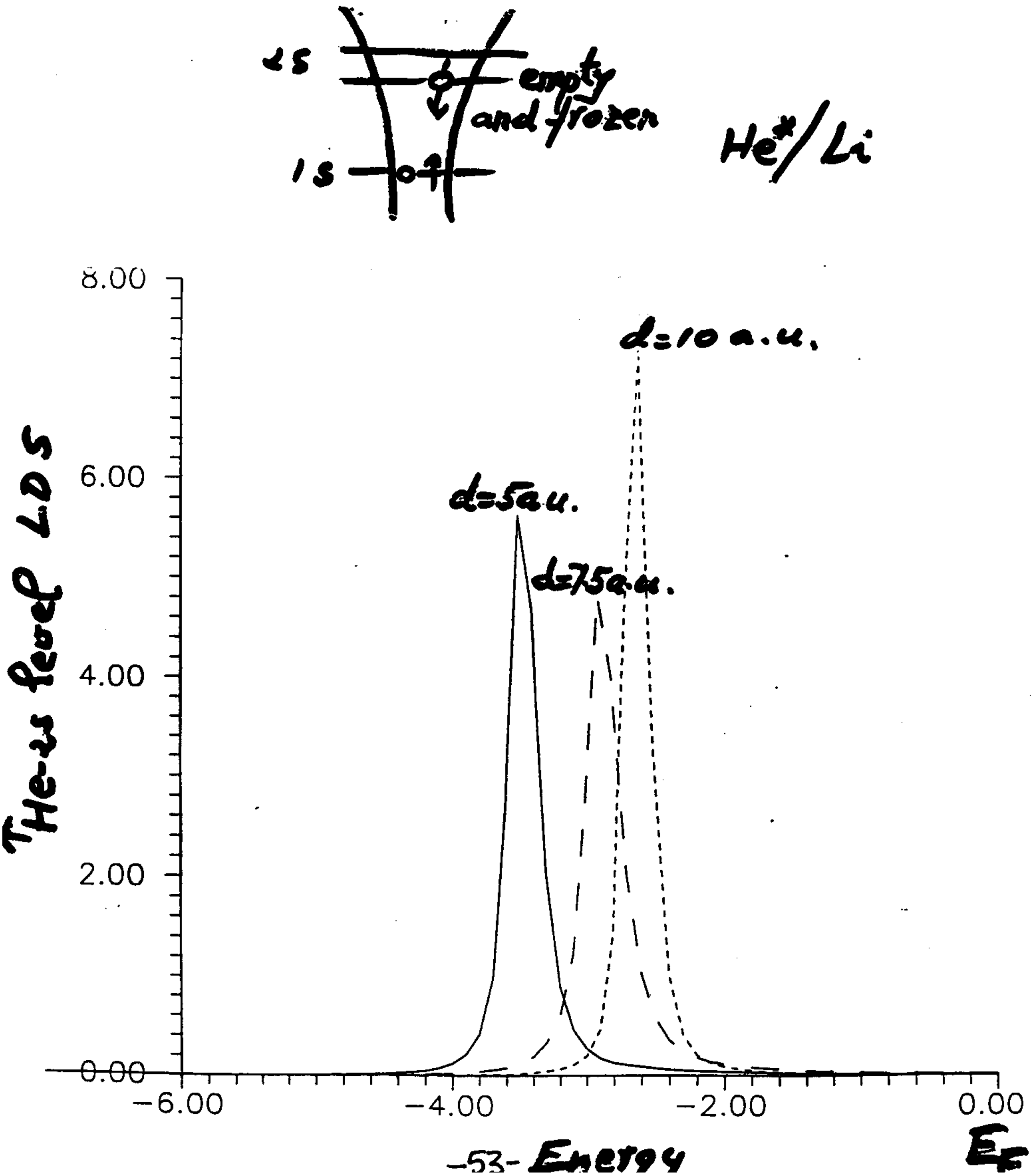


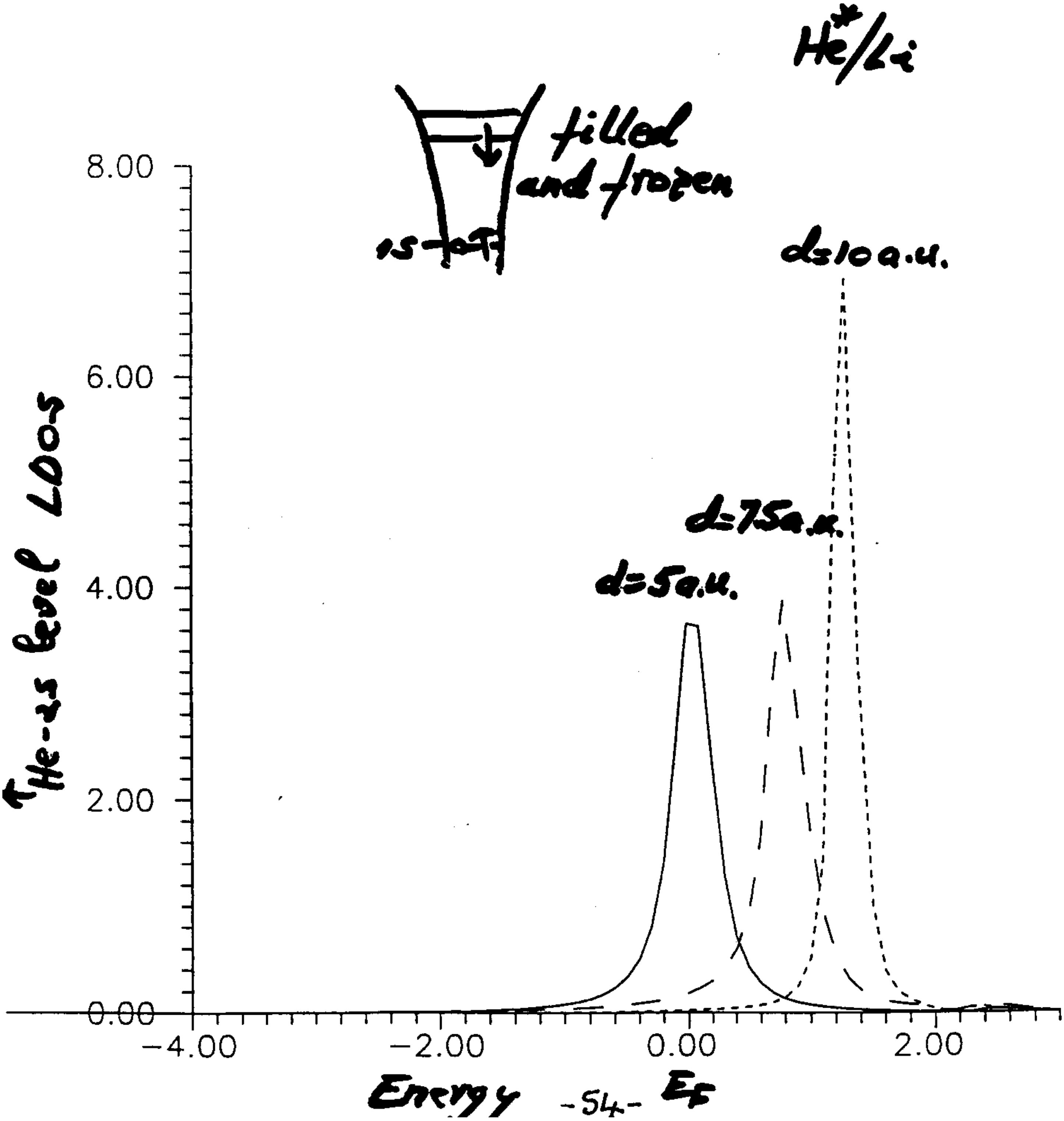
(b)

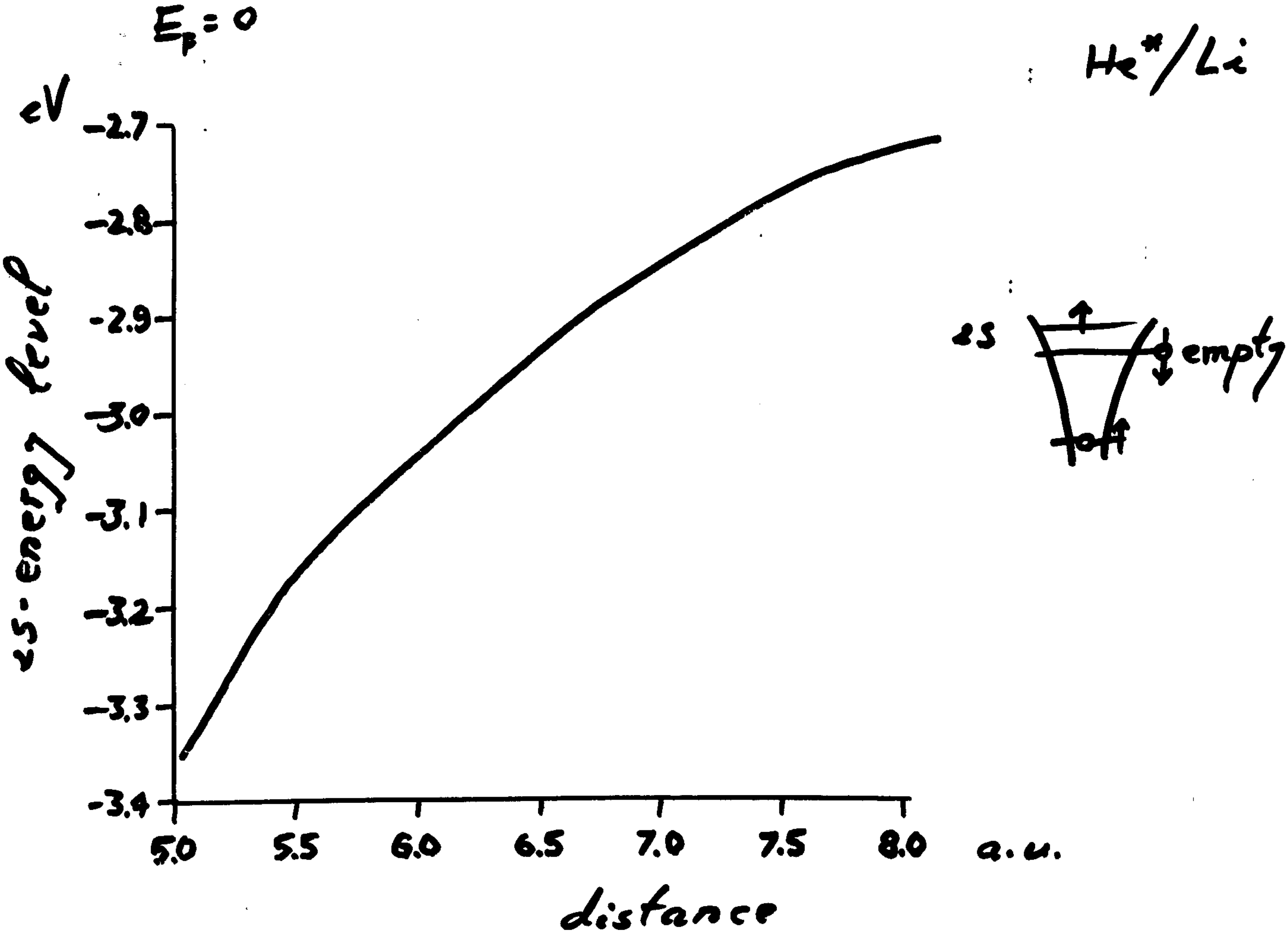


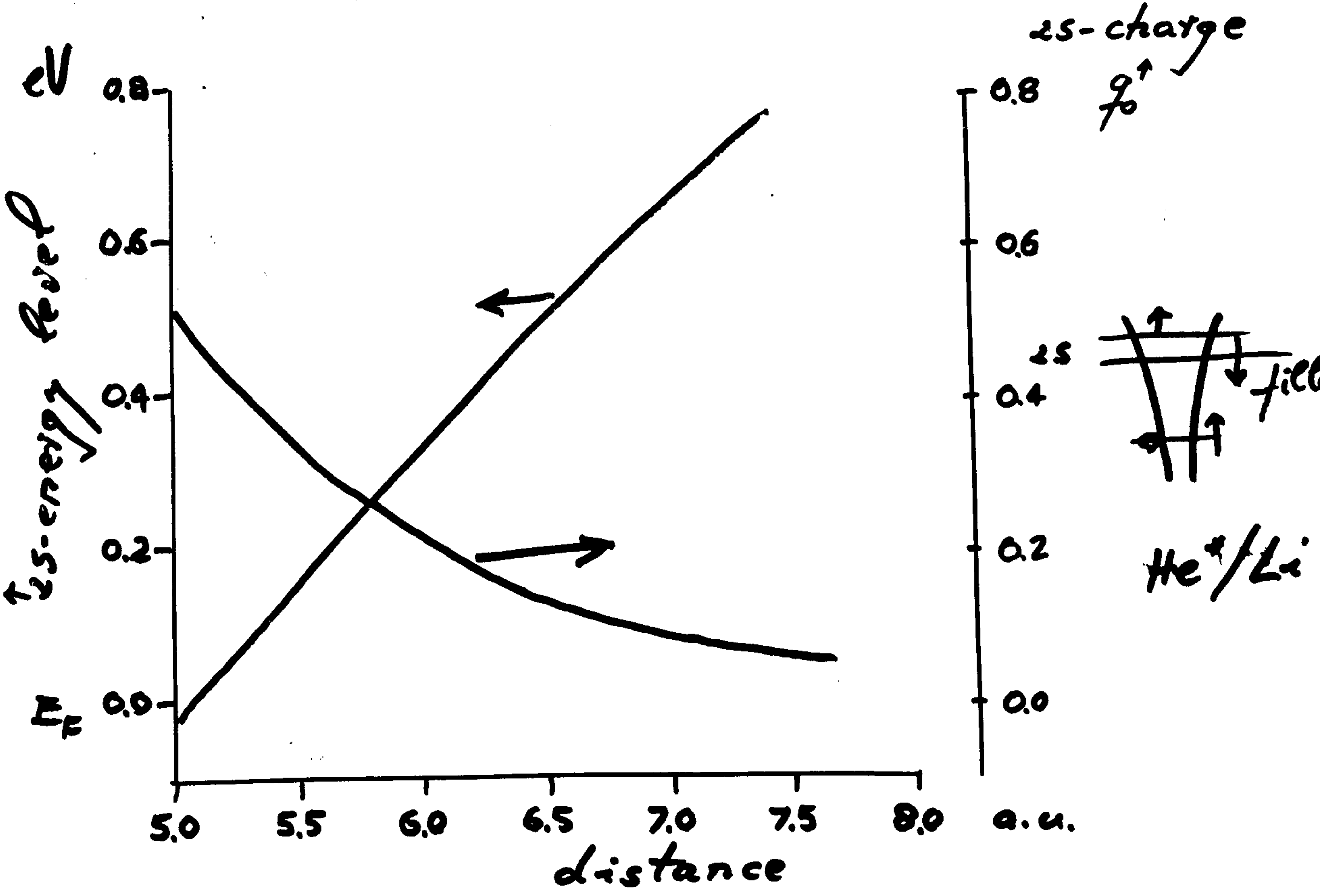
(a) Very low probability process

(b) Defines the dominant me-


2s
1s
empty
and frozen
He*/Li
d=10 a.u.
d=5a.u.
d=7.5a.u.
THe-2s level LDS
8.00
6.00
4.00
2.00
0.00
-6.00
-4.00
-2.00
0.00
Energy
EF

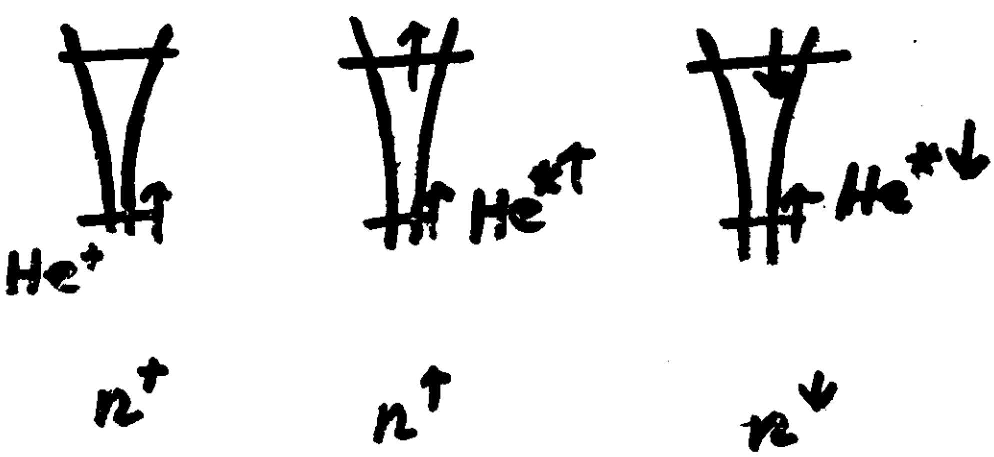

He*/Li
filled and frozen
1s
d=10 a.u.
d=7.5 a.u.
d=5 a.u.
8.00
6.00
4.00
2.00
0.00
-4.00
-2.00
0.00
2.00
π_{He-2s} level LDOS
Energy
E_F


$E_p = 0$
He*/Li
eV
2s-energy level
-2.7
-2.8
-2.9
-3.0
-3.1
-3.2
-3.3
-3.4
5.0
5.5
6.0
6.5
7.0
7.5
8.0
a.u.
distance
2s
empty


eV
1s-energy level
E_F
0.8
0.6
0.4
0.2
0.0
5.0
5.5
6.0
6.5
7.0
7.5
8.0
a.u.
distance
1s-charge
$\varrho_0^{\uparrow}$
1s
fill
He^+/Li

He^*- deexcitation and He^+- neutralization. Resonant processes

He-states



Rate eqns:

$$\frac{dn^{+}}{dt} = \frac{1}{\tau_L^{\uparrow}} n^{\uparrow} + \frac{1}{\tau_L^{\downarrow}} n^{\downarrow} - \frac{2}{\tau_c^{+}} n^{+}$$

$$\frac{dn^{\uparrow}}{dt} = \frac{1}{\tau_c^{+}} n^{+} - \frac{1}{\tau_L^{\uparrow}} n^{\uparrow}$$

$$\frac{dn^{\downarrow}}{dt} = \frac{1}{\tau_c^{+}} n^{+} - \frac{1}{\tau_L^{\downarrow}} n^{\downarrow}$$

Take:

$$\frac{1}{\tau_c^{+}} = \frac{1}{\tau_0} \rho_0$$

$$\frac{1}{\tau_L^{\downarrow}} = \frac{1}{\tau_L^{\uparrow}} = \frac{1}{\tau_0} (1-\rho_0)$$

$$n^{+} = \frac{1-g_0}{1+g_0}\left\{ 1 - e^{-(1+g_0)s} \right\}$$

$$n^{\uparrow} = \frac{g_0}{1+g_0} + \frac{1-g_0}{2(1+g_0)}\, e^{-(1+g_0)s} + \frac{1}{2} e^{-(1-g_0)}$$

$$n^{\downarrow} = \frac{g_0}{1+g_0} + \frac{1-g_0}{2(1+g_0)}\, e^{-(1+g_0)s} - \frac{1}{2} e^{-(1-g_0)s}$$

$$s = \int_{-\infty}^{t} \frac{dt}{\tau_0(z)}$$

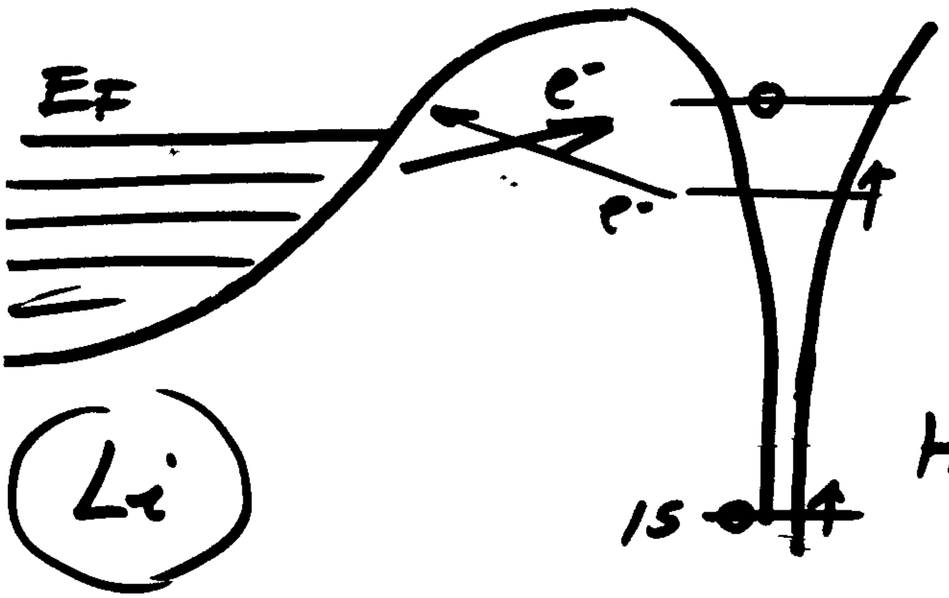
In our case:

$$\frac{1}{\tau_0(z)} = \frac{1}{\tau_0} e^{-\gamma z} \qquad \gamma \simeq 0.72\,a.u.$$

T_0

$$\frac{1}{\tau_0} \simeq 3\,eV \ (6\,a.u.)$$

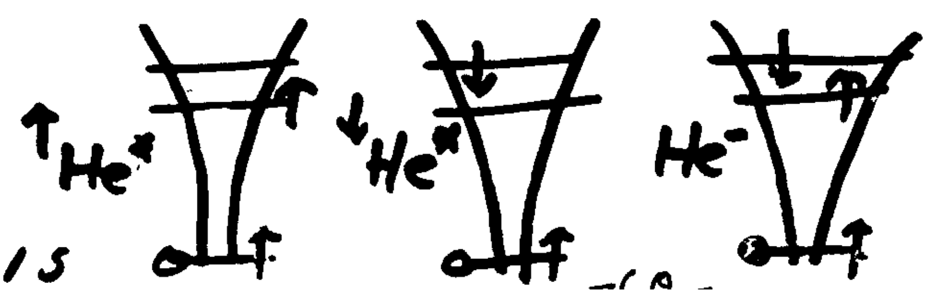
Charge transfer processes: resonant mechanisms (He^*/Li)



$$\begin{cases} {}^{\uparrow}He^* \longrightarrow He^+ & \text{negligible} \\ {}^{\uparrow}He^* \longrightarrow He^- & \text{important} \end{cases}$$

$$\begin{cases} {}^{\downarrow}He^* \longrightarrow He^+ & \text{negligible} \\ {}^{\downarrow}He^* \longrightarrow He^- & \text{important} \end{cases}$$

He-states



Rate eqns (He^{4}/Li):

$$\frac{dn^{-}}{dt} = \frac{1}{\tau_c^{\uparrow}} n^{\uparrow} + \frac{1}{\tau_c^{\downarrow}} n^{\downarrow} - \left(\frac{1}{\tau_L^{\uparrow}} + \frac{1}{\tau_L^{\downarrow}}\right) n^{-}$$

$$\frac{dn^{\uparrow}}{dt} = \frac{1}{\tau_L^{\uparrow}} n^{-} - \frac{1}{\tau_c^{\uparrow}} n^{\uparrow}$$

$$\frac{dn^{\downarrow}}{dt} = \frac{1}{\tau_L^{\downarrow}} n^{-} - \frac{1}{\tau_c^{\downarrow}} n^{\downarrow}$$

Here:

$$\frac{1}{\tau_c^{\uparrow}} = \frac{1}{\tau_0} g_0^{\uparrow}$$

$$\frac{1}{\tau_c^{\downarrow}} = \frac{1}{\tau_0} g_0^{\downarrow}$$

$$\frac{1}{\tau_L^{\uparrow}} = \frac{1}{\tau_0} (1 - g_0^{\uparrow})$$

$$\frac{1}{\tau_L^{\downarrow}} = \frac{1}{\tau_0} (1 - g_0^{\downarrow})$$

(a) Initial conditions:

$n^{\downarrow}=1$ (singlet); $n^{\uparrow}=n^{-}=0$

$$n^{\uparrow} \simeq \frac{g_0^{\downarrow}}{g_0^{\uparrow}+g_0^{\downarrow}}\left(1-e^{-S_2}\right)$$

$$n^{\downarrow} \simeq \frac{g_0^{\uparrow}}{g_0^{\uparrow}+g_0^{\downarrow}}+\frac{g_0^{\downarrow}}{g_0^{\uparrow}+g_0^{\downarrow}}\, e^{-S_2}$$

$$n^{-} \simeq \frac{g_0^{\uparrow} g_0^{\downarrow}}{g_0^{\uparrow}+g_0^{\downarrow}} - \frac{1}{2} g_0^{\downarrow}\, \frac{g_0^{\uparrow}-g_0^{\downarrow}}{g_0^{\uparrow}+g_0^{\downarrow}}\, e^{-S_2} - \frac{1}{2} g_0^{\downarrow}\, e^{-2S_1}$$

$$S_1 = \int_{-\infty}^{t} \frac{dt'}{\tau_0(z)} \quad ; \quad S_2 = \frac{1}{2}\int_{-\infty}^{t} \frac{(g_0^{\uparrow}+g_0^{\downarrow})\,dt'}{\tau_0(z)}$$

$$\frac{1}{\tau_0(z)} = \Gamma_0\, e^{-\gamma z} \qquad g_0^{\sigma} = a^{\sigma} e^{-\gamma' z}$$

(b) Initial conditions:

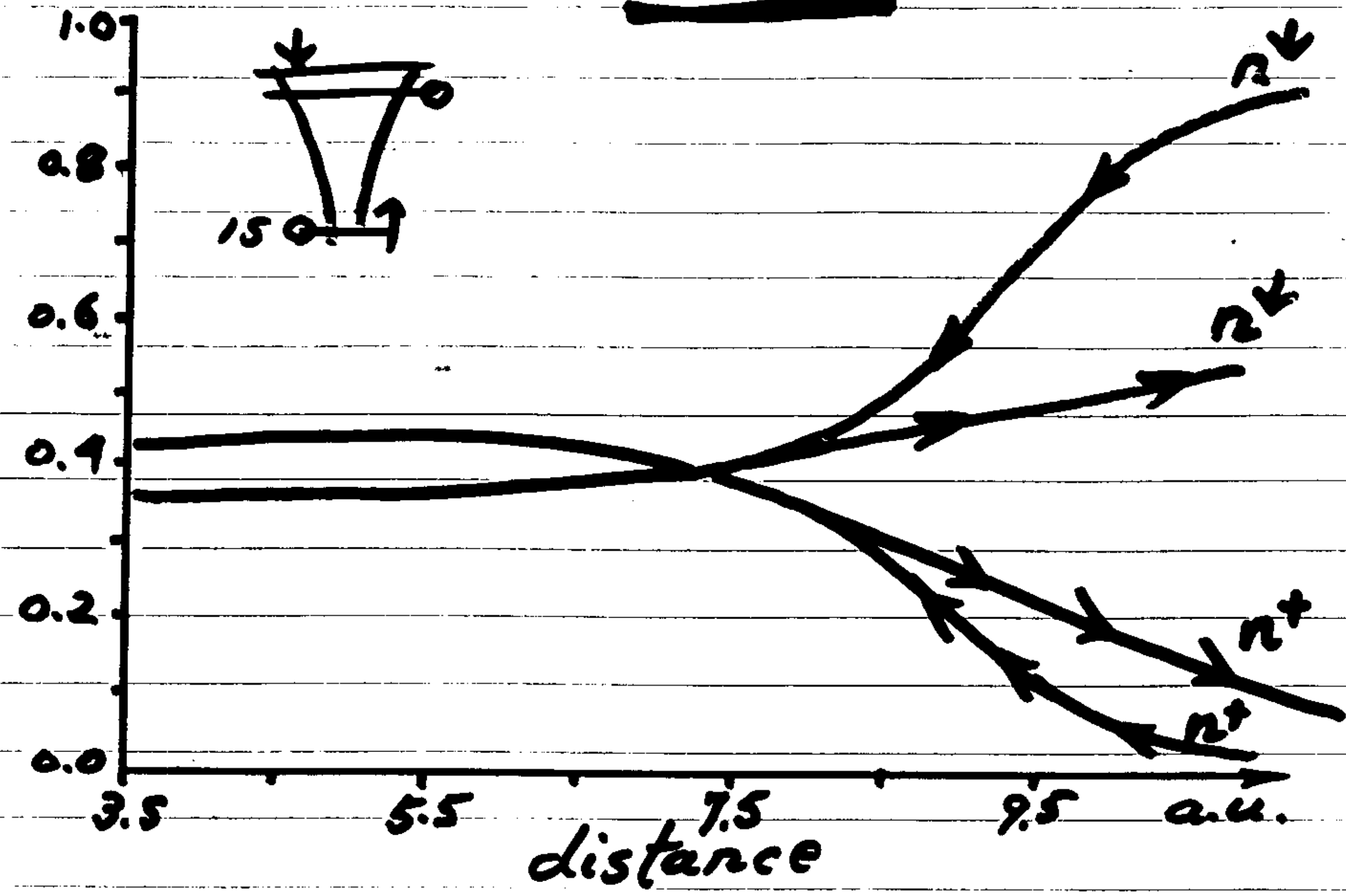
$$n^{\uparrow} = 1 \text{ (triplet)}; \quad n^{\downarrow} = n^{-} = 0$$

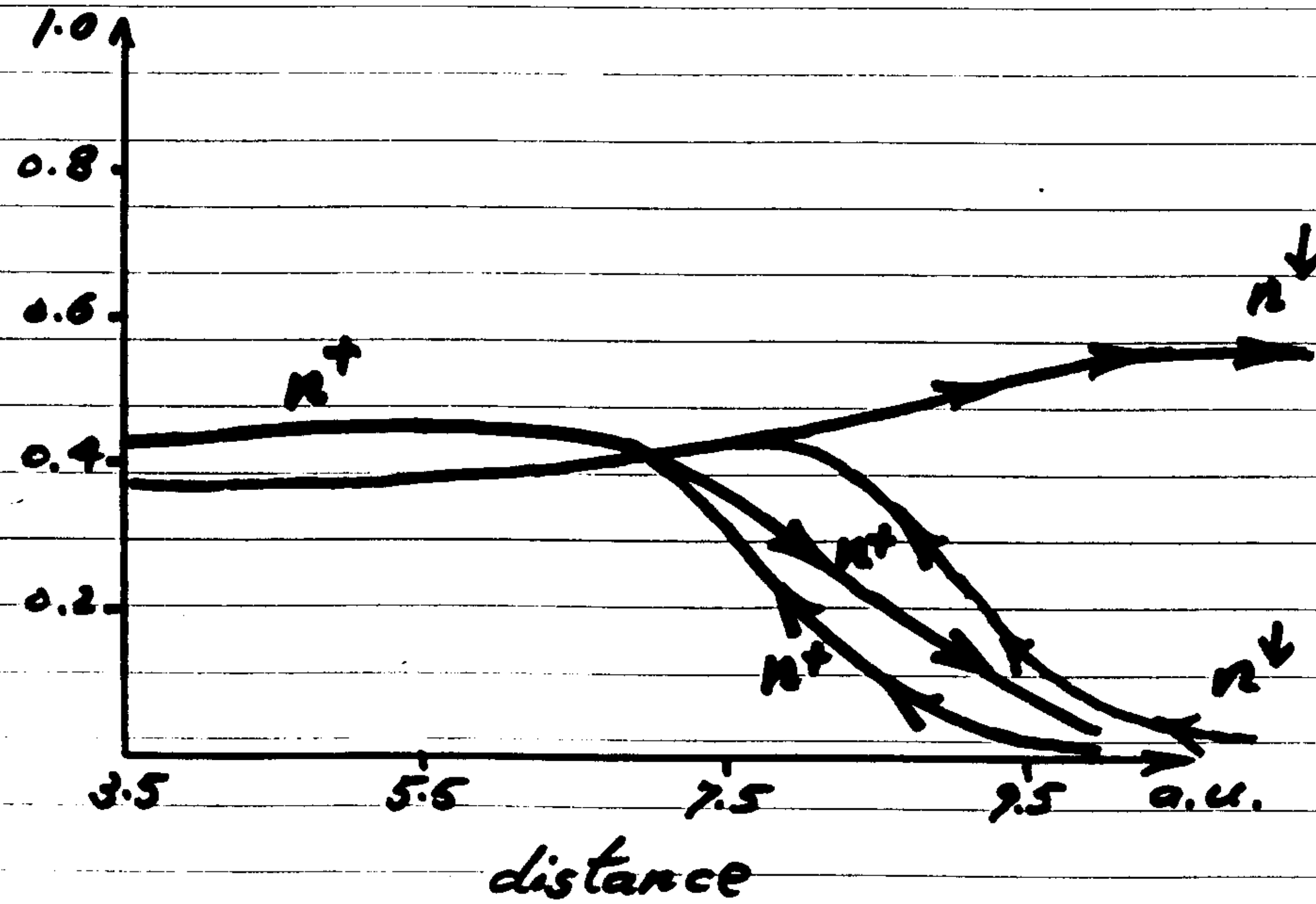
$$n^{\uparrow} = \frac{g_0^{\downarrow}}{g_0^{\uparrow} + g_0^{\downarrow}} + \frac{g_0^{\uparrow}}{g_0^{\uparrow} + g_0^{\downarrow}} e^{-s_2}$$

$$n^{\downarrow} = \frac{g_0^{\uparrow}}{g_0^{\uparrow} + g_0^{\downarrow}} \left(1 - e^{-s_2}\right)$$

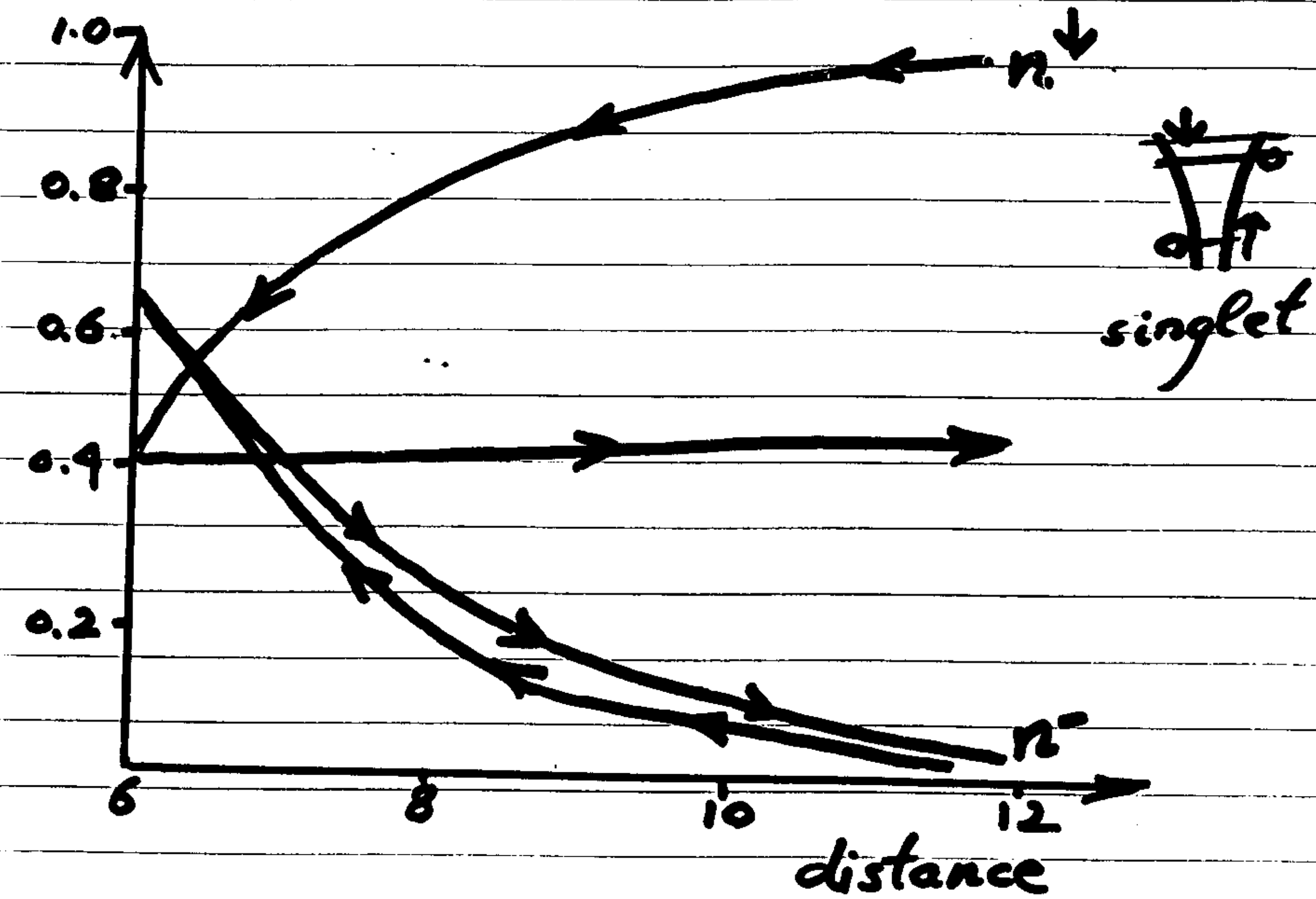
$$n^{-} = \frac{g_0^{\uparrow} g_0^{\downarrow}}{g_0^{\uparrow} + g_0^{\downarrow}} - \frac{1}{2} g_0^{\uparrow} \frac{g_0^{\downarrow} - g_0^{\uparrow}}{g_0^{\uparrow} + g_0^{\downarrow}} e^{-s_2} - \frac{1}{2} g_0^{\uparrow} e^{-2s_1}$$

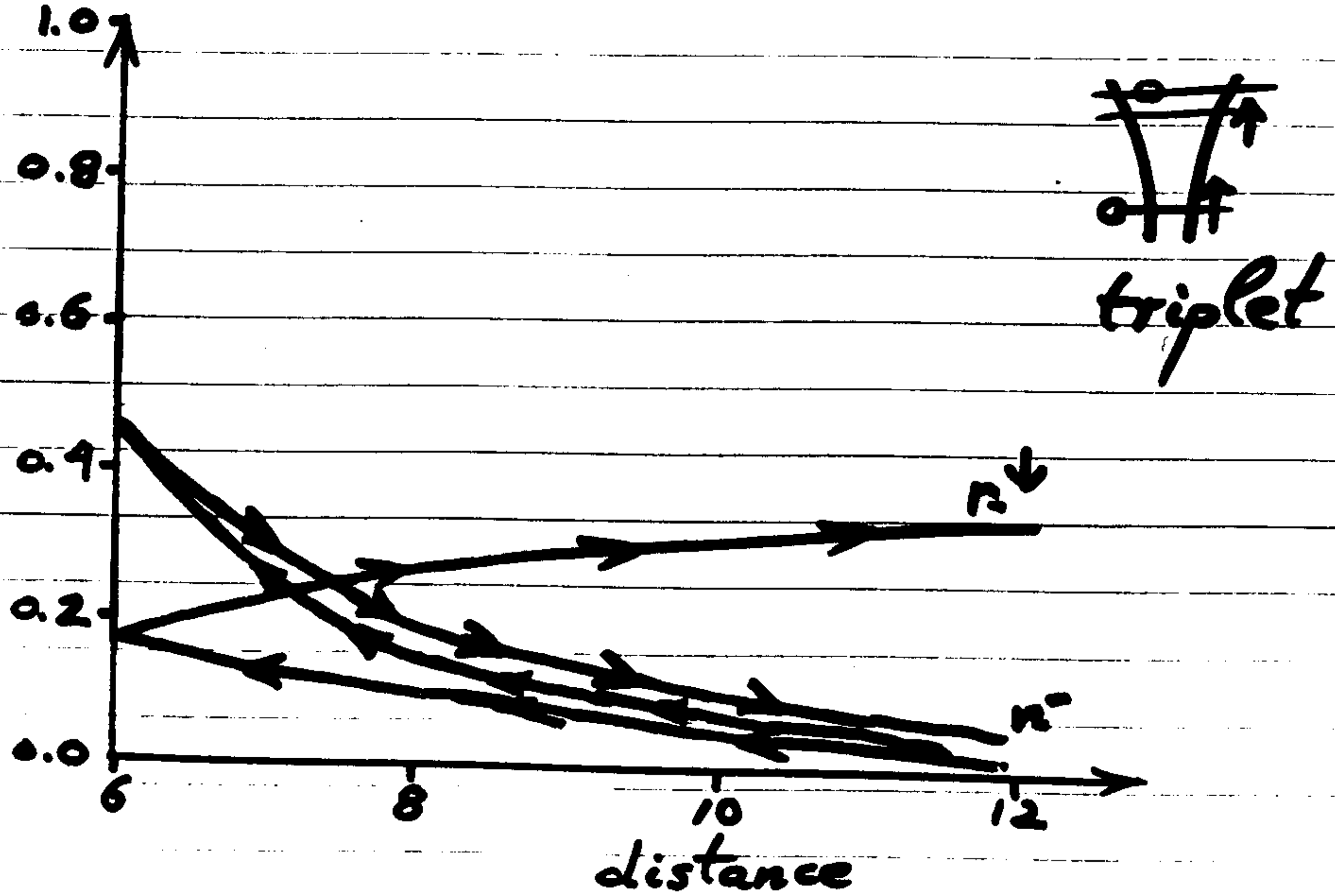
He*/Al





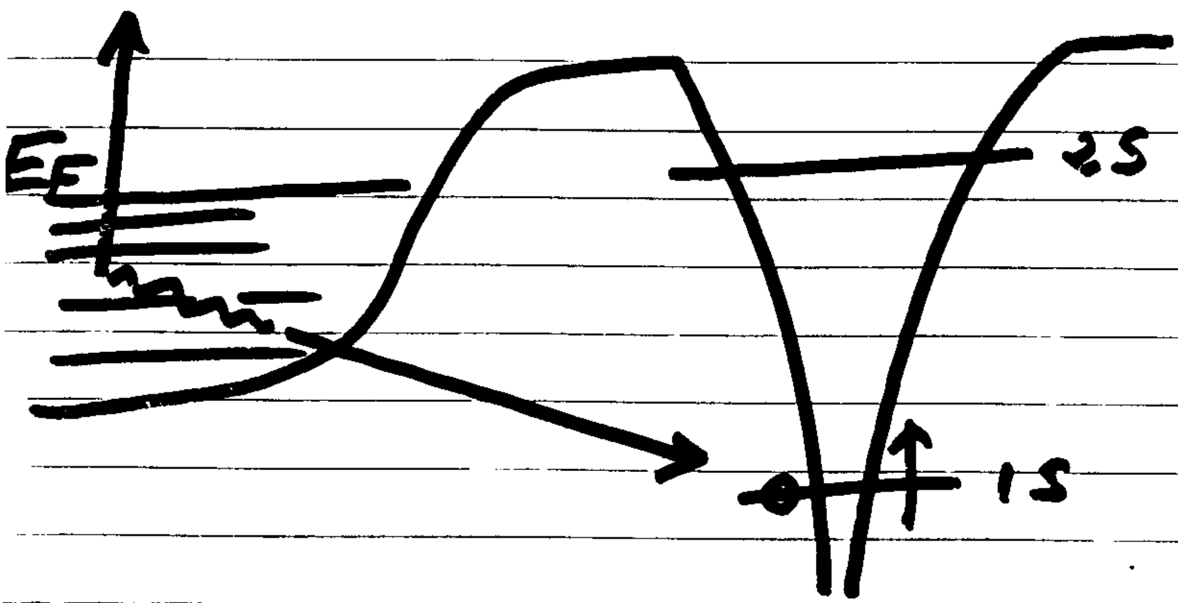
Auger processes neglected



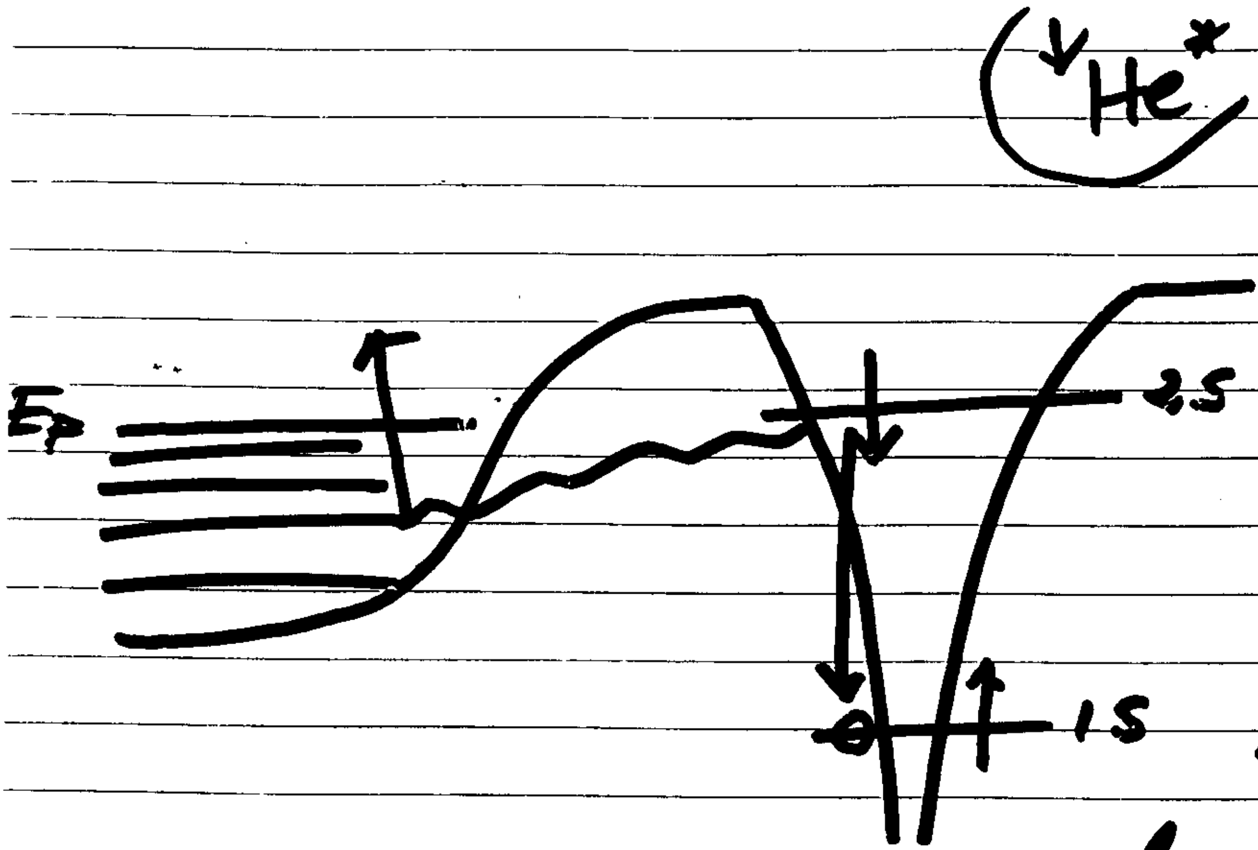


Auger-processes neglected

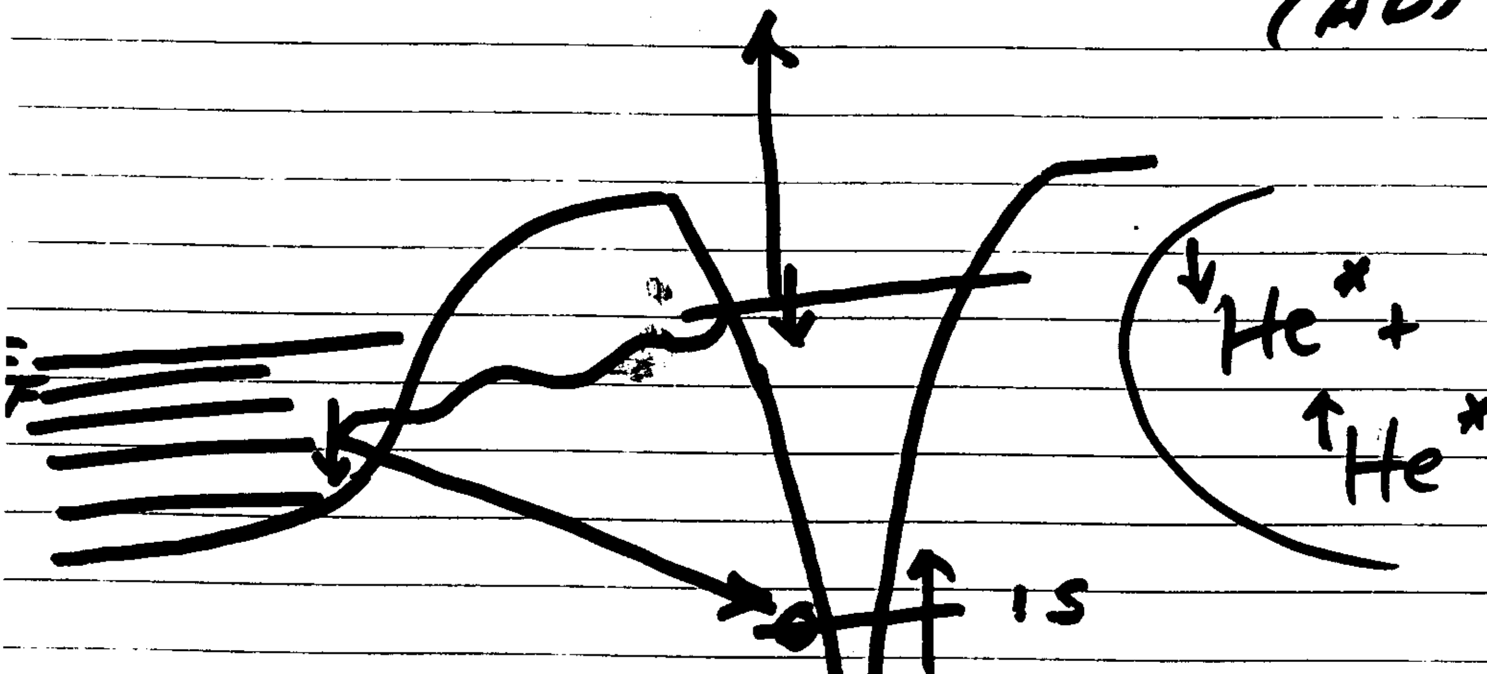
Auger processes



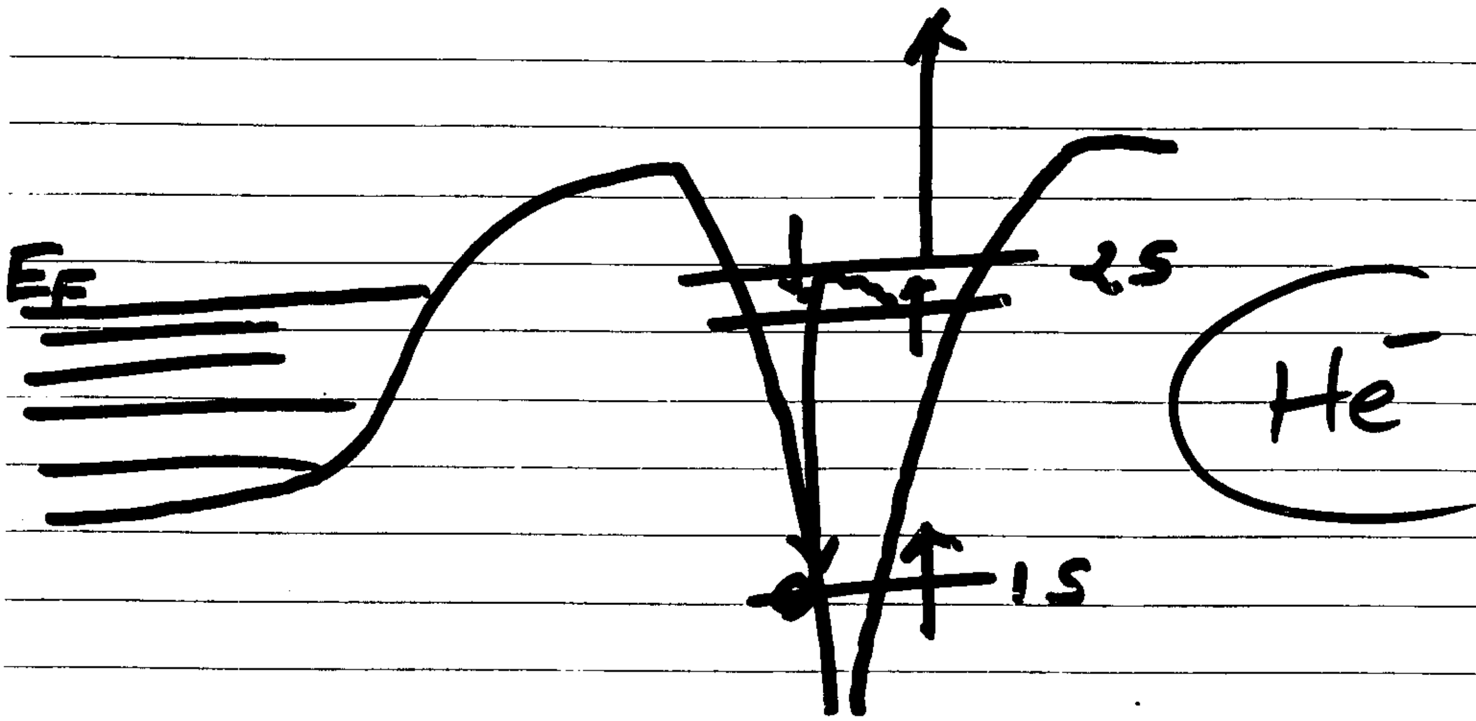
Auger neutralization (AN)



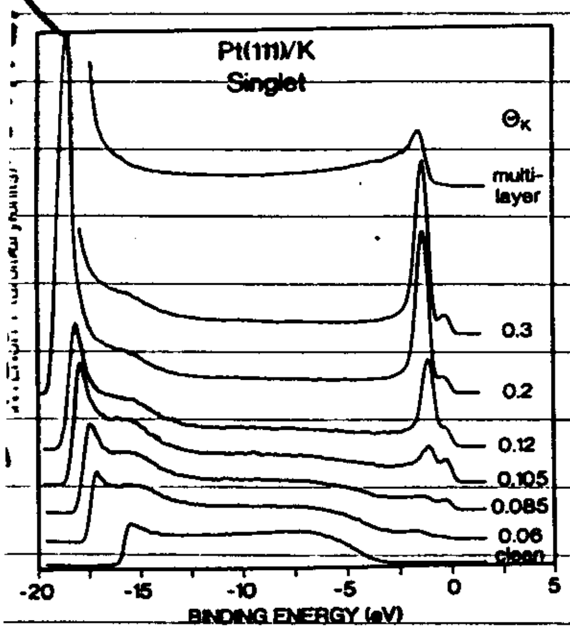
Auger deexcitation (AD)



Penning deexcitation (PD)



Auger autoionization (AA)



IG. 1. Penning deexcitation spectra of K adsorbed on
111).

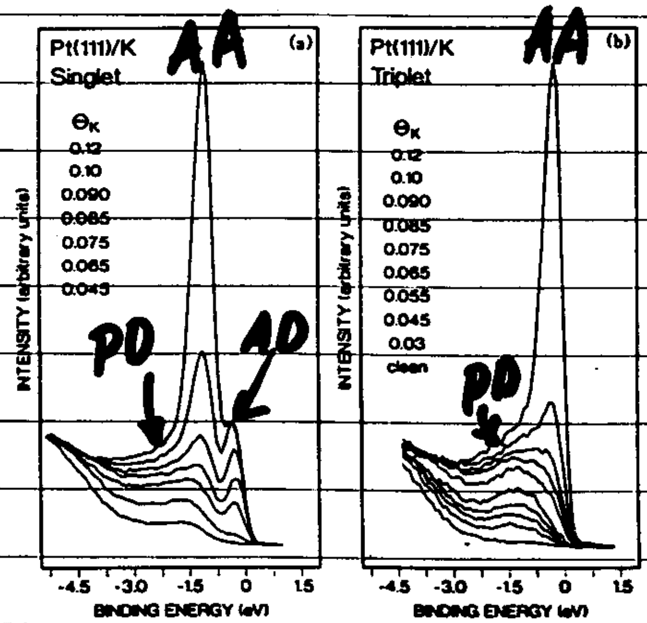


FIG. 2. Penning deexcitation spectra of K adsorbed on Pt(111) from (a) singlet and (b) triplet He* atoms.

Hemmen + Conrad

PRL (1991)

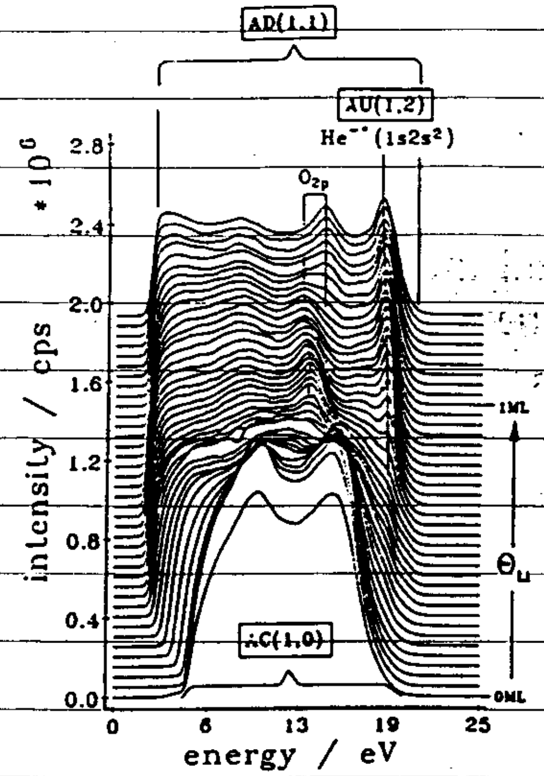
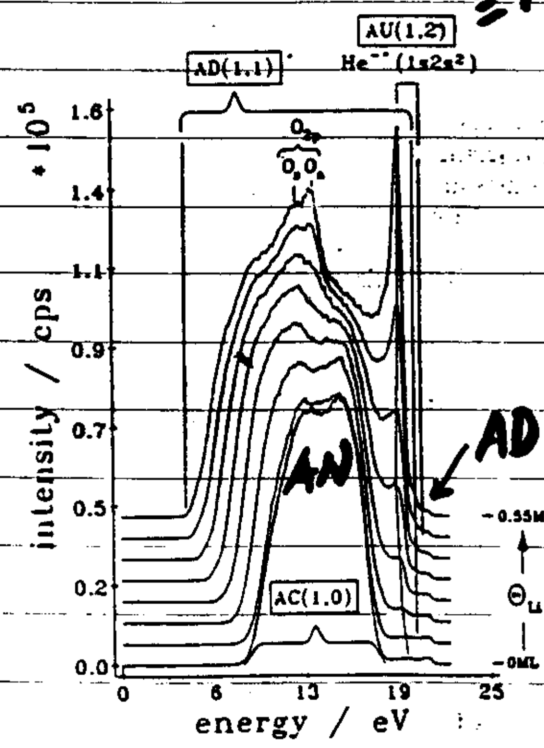


Fig. 1. Electron energy spectra at 8 eV He$^+$ beam energy for collisions with Li(Θ_{Li})/W(110). Incidence angle with respect to the surface $\Phi = 5$ degs; the bottom curve is for $\Theta = 0$ Ml; Θ increases in steps of 0.05 Ml up to one complete monolayer

≡ AA



Brenten et al
Z. Phys. D
(1992)

Fig. 2. Electron spectra for thermal He*(2^3S; 2^1S) atoms colliding with Li(Θ_{Li})/W(110). Incidence angle $\Phi = 45$ degs; the bottom curve is for $\Theta = 0$ Ml; Θ increases in steps of 0.1 Ml up to 0.6 Ml. Data are taken from [30]