[1]N R E L G , C 80201, USA
[2]U E -N , G

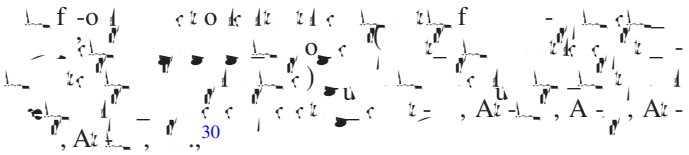
(24 2005; 15 2006; 13 2006)

[illegible]

DOI: 10.1103/[illegible].74.035108 PACS number(s): 61.66.[illegible], 61.50.A[illegible], 81.05.[illegible], 81.30.[illegible]

I. INTRODUCTION

[illegible]



$$\Box H_{LDA}\left(\Box\right) \equiv E_{\left(\Box,V_{\Box},\{\mathbf{R}_{x}\right.}$$

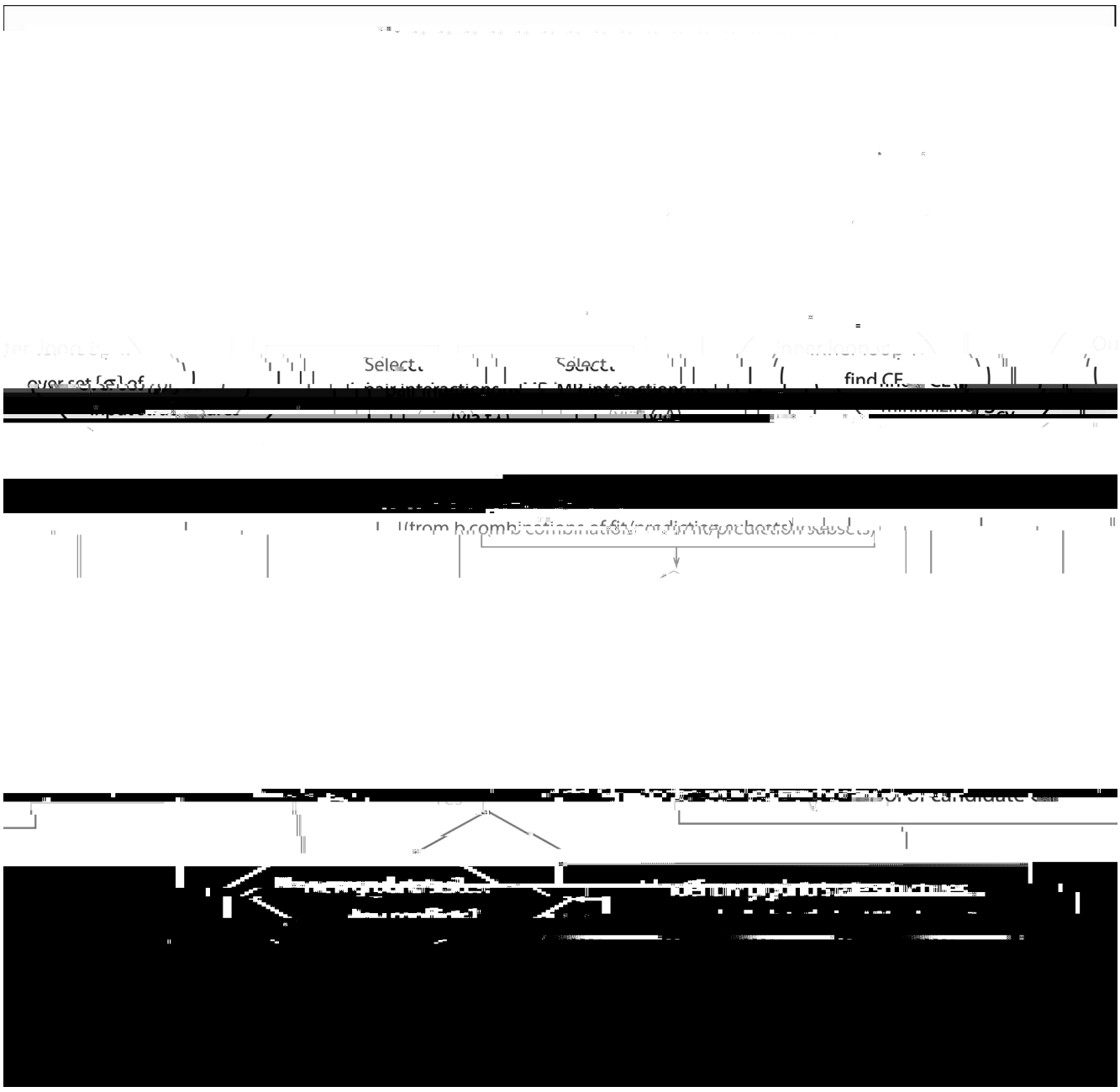


FIG. 3.

$$D_{J_{\alpha\beta}}(\omega) = \sum_{\alpha\beta} J_{\alpha\beta} |S_{\alpha\beta}(\omega)|^2, \quad (7)$$

$$\text{MBCE} = \sum_{\omega \in \text{ol}} |H_{\text{LDA}}(\omega) - H_{\text{CE}}(\omega)|^2 + M, \quad (8)$$

$$M = \frac{1}{\square} \quad J_{(})[\ \nabla^2]^{\square/2} J_{(}) = \overset{\circ}{} R^{\square} D\ J^2 \qquad (9)$$

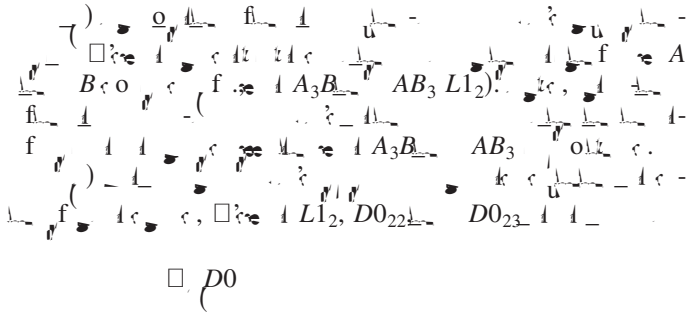
8)

. A . . A 1 o □H_{LDA}) A 1 x x o □H_{CE} o. A f o □H_{CE} □H_{CE} .

x				□H_{CE}	□H_{LDA}		□H_{CE}
		o 2					
1/9	A_8B	301) A_8B	.	45.1···	38.5	39.4	38.6
1/6	A_5B	301) A_5B	.	59.5···	55.9	57.4	57.3
1/5	A_4B	201) 301) A_4B	.	71.3···	67.9	67.3	67.3
5/12	A_7B_5	302) $A_2B_2A_3B_2A_2B$	.	91.3···	89.1	93.7	93.7
		o 3					
1/5	$A_{12}B_3$	301) A_5BABA_6B	.	71.0···	67.9	67.5	68.5
4/15	$A_{11}B_4$	401) A_5BABA_4BAB 2 , f . 14)	.	86.6···	84.9	85.4	85.7
2/5	A_9B_6	401) $A_4B_4A_4BAB$	.	92.9···	91.6	93.6	89.5
2/3	A_4B_8	302) $B_5A_2B_3A_2$	.	69.0···	63.2	58.7	62.4
	A_2B_4	301) A_2B_4	.	68.6···	66.4	59.1	58.4
		o 4					
2/11	A_9B_2	301) A_5BA_4B	.	64.9···	62.3	62.5	63.9
1/3	$A_{10}B_5$	401) $A_4BABA_2BA_2BAB$	.	91.9···	87.8	87.8	87.9
	A_8B_4 (. 4905)	302) $A_5B_2A_3B_2$	.	95.7···	85.4	91.1	88.2
2/5	A_3B_2	110) A_2BAB	.	94.0···	86.7	89.4	89.8
5/8	A_3B_5	401) B_4A_2BA	.	75.6···	68.2	64.1	66.6
2/3	A_4B_8	601) B_6ABA_2BA	.	68.2···	61.6	60.7	59.7
		o 5					
1/6	$A_{10}B_2$ (_)		.	62.2···	54.2	55.3	55.3
1/5	A_8B_2 (_)		.	71.5···	66.5	66.5	67.4
1/3	A_8B_4 (. 4557)	$A_3BA_2BA_3B_2$ 201)	.	91.2···	88.8	91.1	90.4
7/12	A_5B_7	302) $B_2A_2B_3A_2B_2A$	.	94.4···	91.9	74.8	77.2
		o 6					
1/9	$A_{18}B_2$ (_)		.	37.9···	34.8	34.4	35.0
2/17	$A_{15}B_2$	401) $A_{14}BAB$	.	43.0···	41.4	41.0	41.3
4/17	$A_{13}B_4$	401) A_6BABA_5BAB 2 , f . 14)	.	81.5···	78.9	79.9	80.4
1/2	A_3B_3 (. 55)	111) A_3B_3	.	41.3···	7.4	11.6	11.7
		o 7					
1/11	$A_{10}B$	301) $A_{10}B_1$	.	32.7···	31.7	31.4	32.2
2/13	$A_{11}B_2$	301) A_6BA_5B	.	54.7···	53.2	53.3	54.6

I . E AND RANGE F IN EAC I ON REQ7 IRED F R DE CRIBING L

A 3 $L1_2$) f , o □ □) □=$L1_2$, $D0_{22}$, $D0_{23}$) 12 o 2 - f $L1_2$- A 3 $D0_{23}$) A 3 $L1_2$) f , o □ □) □=$L1_2$, $D0_{22}$, $D0_{23}$) 12 o 2 - f):



B. t : t f st t s f st t t CE

1. Ground-state search at different outer-loop iterations

f . 10 f =7). (o =1 =7). f o 16 =1) o 20 (=7) , f f

A k : f o , A f . 10)] f $\square H_{CE}$ ( )f ( ) f f / $\square$ $\square$)=0 A. f . 3) . 40% 96 -49-

f . 4, f o o f f o f . 9). =1, o o f , f o o f . f f o

the82ed92.0693n Tf 298.6
the7n2203.1556n Tf 29.5
N96 -90T5dicatesN96 -89
155 041o951 29.5037.015 298
0%85 $\square$) 21.3499 29599
1684 1236951 3458 1.37.015 2
18 88 4458 1.37.015 29
193 95 -0.05458 1.37.015 29
96 -43.19.26285 /
0%5.5 21.3499 29599
A/.89 8458 1.37.015 298
4.10092220 -519

x ( ) $\square H_{CE}$ f ( ) $\square H_{LDA}$ ( )

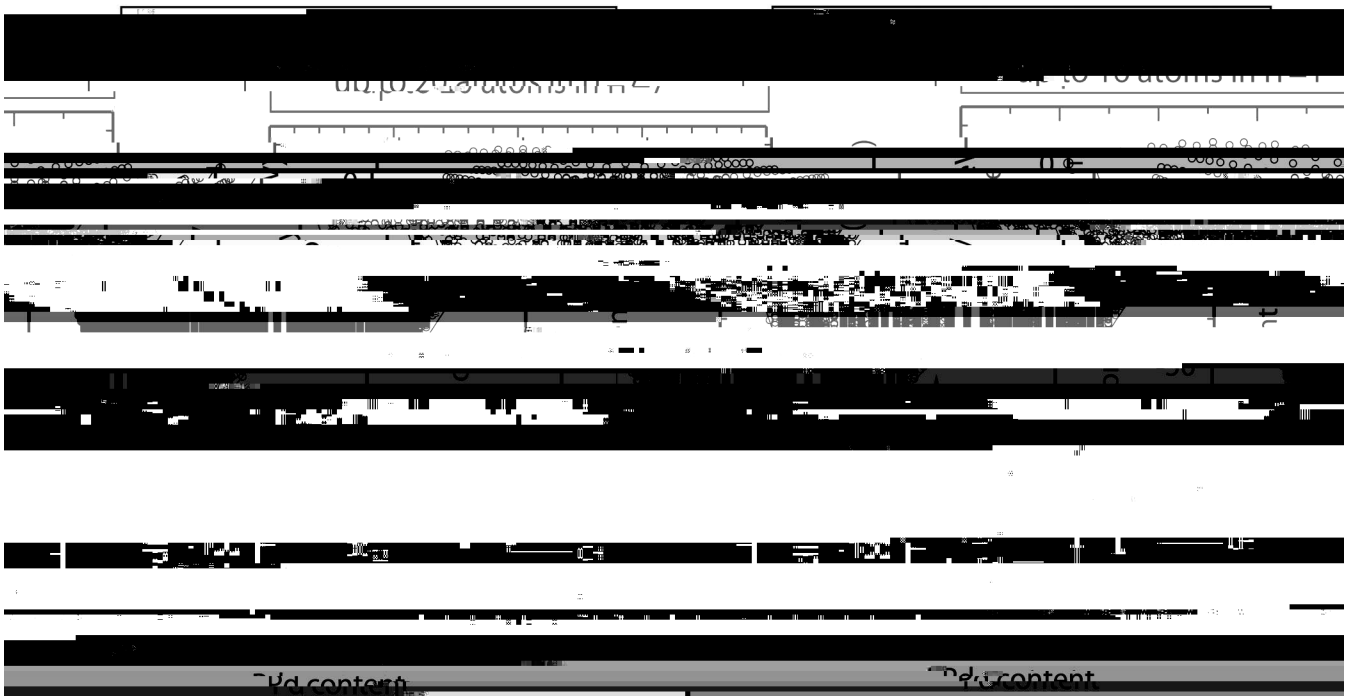


FIG. 10. ( ) =1 ( )=7 ( ). Al f .

o); f f =1.

2. Illustrating the outer-loop history

f ( ) o A f . 11 f , oo f f o A), f ; f o), f f A (f o A f . 11, f =1 f . 11 o =1 ( ) f o A=1. f .) *CE* *LDA* o- f A2 1 A2 2 A 1 A f o .) *CE* *LDA* . *L*1$_2$- o =1), A f o f (.) *N* - o f A8 [301)$A_8B_{\ }$], A5 [301)$A_5B_{\ }$], A4 [301)$A_4B_{\ }$] A7 5. =1 f f . 11 A o .

A *L*1$_2$- f -o o A3 A3 *L*1$_2$- o.

o	:	*N*=28 =1	*N*=32 =2	*N*=37 =3	*N*=43 =4	*N*=47 =5	*N*=51 =6	*N*=53 =7
A3	A- f ($D0_{23}$)	0%	88%	92%	62%	64%	100%	100%
A3	A *L*1$_2$/*D*0$_{22}$/*D*0$_{23}$	0%	88%	92%	62%	64%	100%	100%
A3	A- f (*L*1$_2$)	40%	100%	100%	92%	79%	100%	100%
A3	A *L*1$_2$/*D*0$_{22}$/*D*0$_{23}$	0%	37%	100%	85%	79%	100%	100%

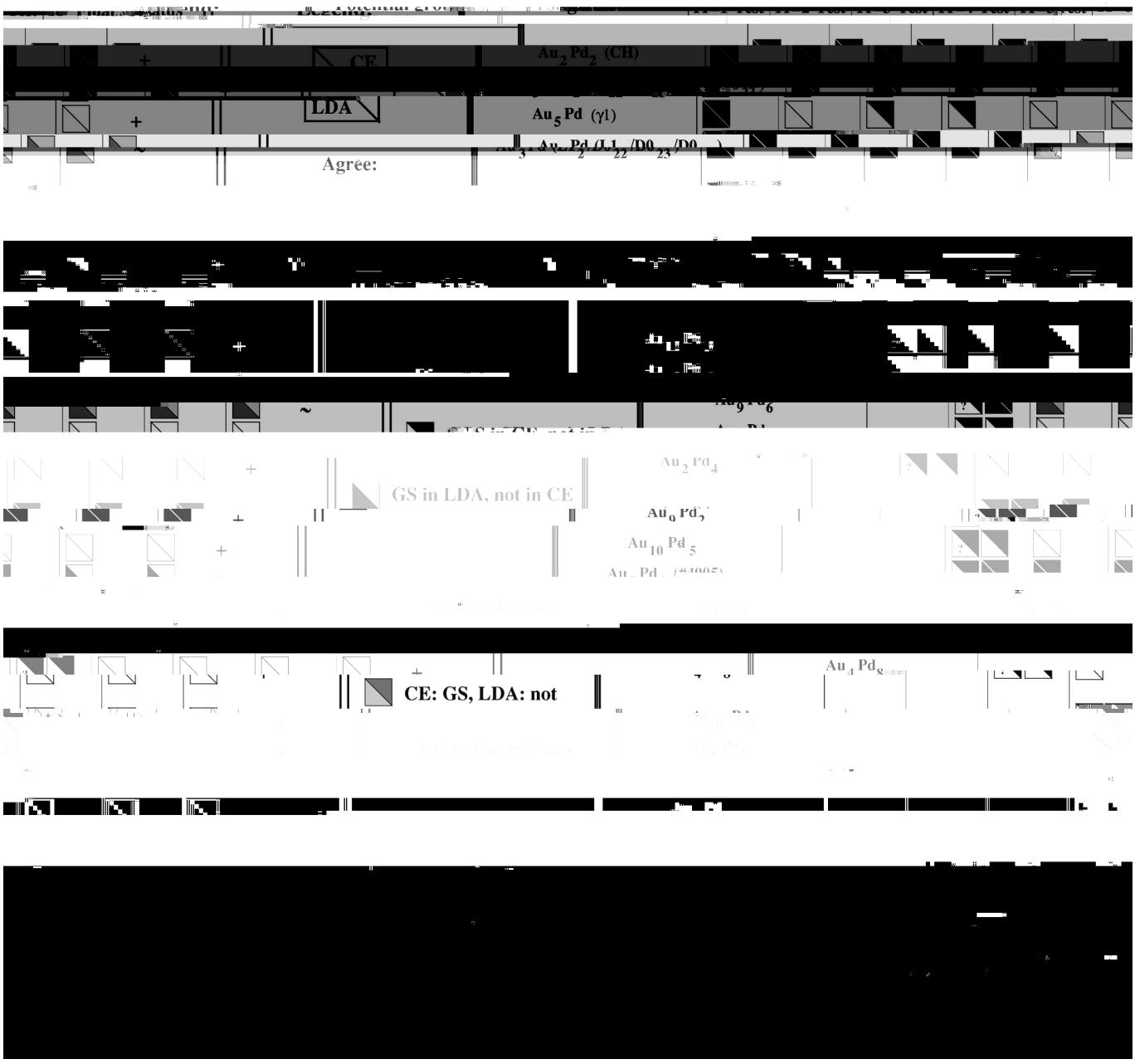


FIG. 11.

f .

) *CE* *LDA*
A

) *CE* *LDA* A

) S *LDA*

ΔH_{LDA}

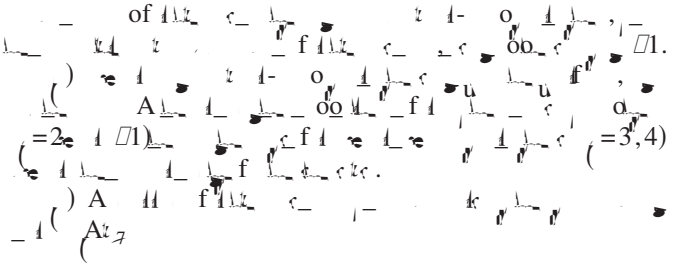
(1)

3. Generic behaviors during outer-loop iterations

f . 11,

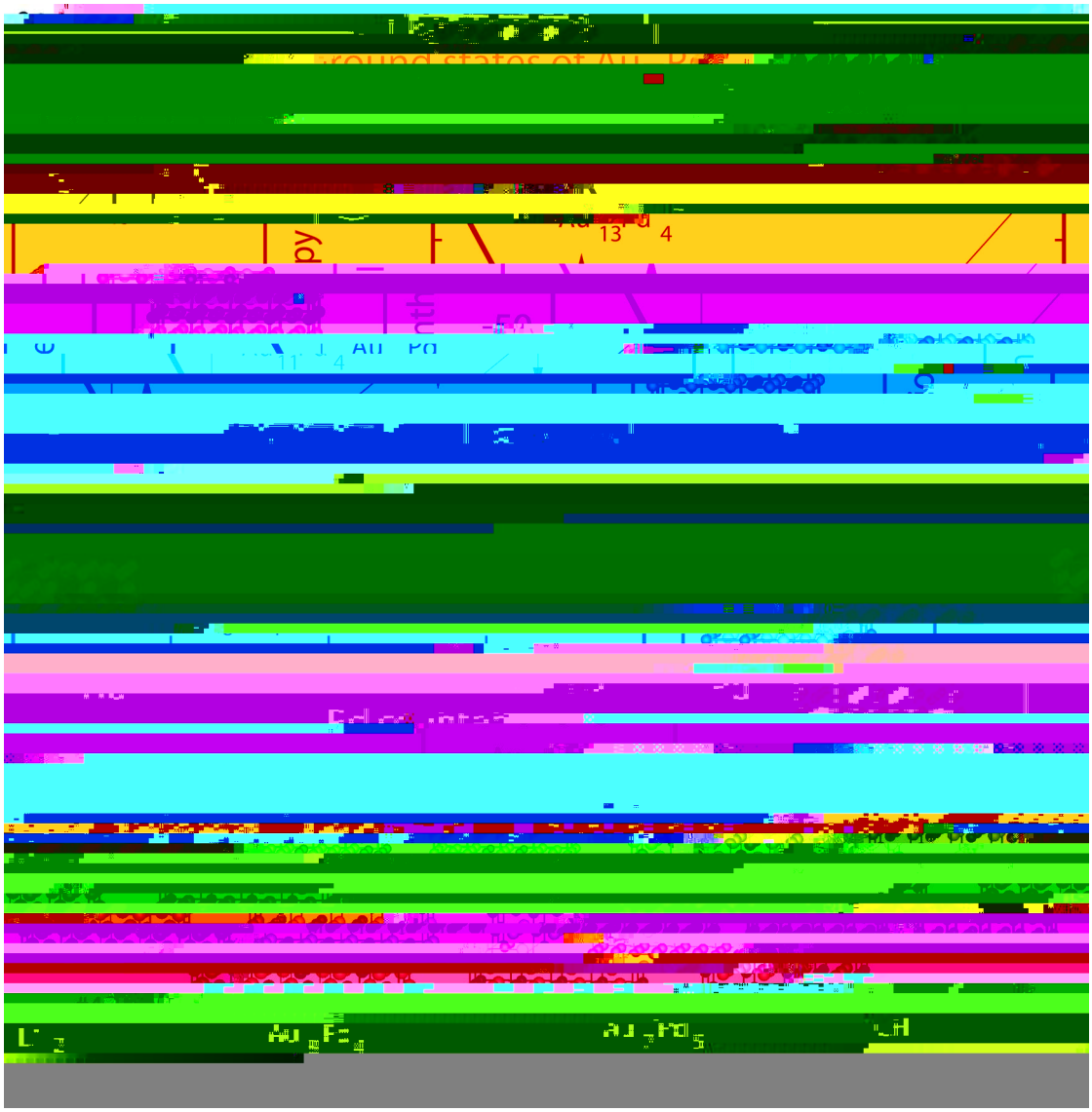
) A

) A



II. DI C7 I N F G R 7 ND- A E RDERED- R7 C 7RE IN A 1 x x

A. - A 1 x x m s, x 0.22: (301) “ t st t s



G. 14. ( ) x 0.22 f . 10)] oo A (f .

f o) (40 f 57). f A 1 x x=1/2 15 : f f , 8 f o , f 89 90 , 91 A) (0 f o f o f o / f f o f .

A o f 5 - f f f), f) J 0,) J 0,) J 1, D0 22 A5B f . f f A - , f o f .

E. D t m s st s : E st t st f -f st t s A -

, o 15,53 f f f f f .

III. CONCLUSION

[78] [illegible]

[79] [illegible] (Ann. Math. **30**, 244 (1944)).

[80] [illegible]

[81] [illegible] (см. D0$_{23}$ [illegible] $L1_2$ [illegible] D0$_{22}$. [illegible] D0$_{23}$ [illegible] $L1_2$123