PHYSICAL REVIEW B VOLUME 26, NUMBER 2 15 JULY 1982

Quasiband crystal-field

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I. INTRODUCTION

Substantial progress has been made over the past
few years in advancing the

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II. STATEMENT OF THE PROBLEM

Our description of the problem addressed in this
paper consists of (1) a formulation of the host- (H)
crystal problem, (2) the definition of the potential
perturbation associated with the defected (D) crys-
tal, and (3) the statement of the defect problem. In this section we define the basic quantities appear-ing in the forthcoming discussions and in the pre-sentation of our method.
The electronic structure of the ideal host is ex-pressed in terms of a single-particle equation that provides the host wave functions PJ~(k, r) and band
p

energies eJ(k) for a translationally invariant host-crystal potential VH(ptr(r)):

[, V +VH—

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The term e„,[p] is the exchange (with an exchange
coefficient a„) and correlation energy per particle
of the homogeneous electron gas.
Equations (1)—(8) define the electronic structure
of the host crystal; given VH'(r) and N, alone,
one can solve for the self-consistent

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that of atomic dimensions. This analysis

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equations:

g [5,,—QG (e;),,-&g,-

l

b, Vl g, &]C~,——0,

where the

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range part of the perturbing potential is frequently
too strong to permit low-order perturbation ap-
proaches based on the host wave functions as
zero-order states. ' '
Most of these difficulties associated with solving
the deep defect problem are overcome by the

Green's-function approach. ' The knowledge of P;(

r

) only in the range where the perturbing po-

tential b, V(r) is nonzero is sufficient [c f E.

q.
. (18)]
to generate P;(r) everywhere. Consequently, the energies and wave functions of both localized and extended states can be found by using the localized representation in Eq. (16) if the set

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TABLE I. The calculated defect energy levels of a parabolic perturbation potential EV(r)=K(r —ro) in a silicon free-electron host, comparing the results of the conventional
defect

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(g (r R) ~ ~V(» Rt) ~gb(r Rb)&
[cf. Eq. (17a)] involving three-dimensional, nons-
pherical multicentered functions need tomulticentered

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The first to realize that this is, in effect, a gen-
eralized pseudopotential problem was Phillips

who showed that if one orthogonalizes g;(r) to the
ligand orbitals, the crystal-field problem can still
be solved

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method. It was first used in the context of
Green's-function calculations by Lindefelt.
This k-space summation method simplifies the
calculations enormously: Only a small number of
k

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from atomic potentials and if linear mixing ' '
between input and output b, V(r) is used.
We have overcome this difficulty by using a new
and efficient method developed by Bendt and
Zunger for general self-consistency problems.
This method uses a Newton-Raphson technique with Jacobian updates. It is far more effective than potential mixing, ' '

the Pratt scheme,

Kerker's scheme, or Ferriera's accelerator. '

It
enables the efficient self-consistent solution of the defect problem even with modest computational fa-cilities. The method is described in Sec.V D.

V. THE PRESENT RESOLUTION OF THE DIFFICULTIES

We describe in this section our QBCF approach
to resolving the difficulties described in the preced-ing section. The discussion parallels the structure of Secs. IVB1—IVB4.

A. The

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tions. The common critique of basis set orthogo-
nalization states that the long-range oscillations
introduced by this procedure can penetrate the
domain of b, V(r) without adding extra variational
flexibility. In the generalized crystal-field repre-
sentation, however, the existence of a physical dis-tance scale in the problem —the perturbation radius R,

—allows one to overcome this difficulty easily.

The basis Ig&t (r)

I

is Schmidt orthogonalized
within

a sphere of radius R, such that the orthogo-nalized function vanishes outside R,. All members of the set that are linearly dependent to within

a

prescribed tolerance (i.e.

,

the

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essential for describing transition elements and, at
the same time, results in an involved multiple-
scattering form when an overlapping multicenter
representation is used, becomes diagonal in all but

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in the screening potential [Eqs. (35) and (36)] can be constructed from any given densities pD(r) and pH(r), as described in Sec. V B2. A self-consistent solution to the defect Green's function Eqs. (17) and (18)

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(33), (35), and (36). The process is iterated until
the

t

TABLE IV. Convergence of the energy e, (in eV) and orbital-density localization q; of Eq. (44) {in electrons) of the silicon vacancy gap level with respect to the number Mb of host-crystal bands and the number X~ of atoms in a supercell. Also shown is the smallest distance d between adjacent vacancies in neighboring supercells. In Eq. (44), R,=4.44 a.u. (the nearest-neighbor distance). The zero of energy is the valence-band maximum. The basis set consists of 14 radial Coulombic functions with Z =10 for each of the I com-

ponents used (1=1,2, 3,4). The maximum value q

can attain equals the occupation of the t2
level, i.e., 2.0.

Interdefect
distance

d (a.u.) Atoms/cell

Mb ——10 bands

t2

Mb ——21 bands

t2
q;

Mb ——30 bands
t2

q;

21.8
36.3
50.8
65.3
79.8

54
250
686
1458
2662

1.227
0.906
0.817
0.802
0.798

0.48
0.66
0.66
0.66
0.66

1.061
0.715
0.632
0.610
0.604

0.66
0.70
0.70
0.70
0.70

1.025
0.682
0.602
0.

682

0.

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k,,='0.66(0,0,1)
d,,=6

I t

k,,=0.3$(1,1,1)
cI, =8

VB CB CB

t~

CV:

~O
O
o

l

0

IK,,=(0,0,0)
d, =1

k,,=066{0,1,1)

VB CB —VB CB

w

10

.I.

15

L.. l
20

BAND INDEX j

l I

10 15 20

FIG. 2. Spectral decomposition of the t2 gap-state wave function f; (r) of the silicon vacancy in terms of host-t2 crystal Bloch wave functions PJ {k,r). The coefficients are given by P; (r)= g.

7 Td7g.

t BT /i21 8.24 Tf 69.0 Td6.01 302. (37 7 711.BT /T /Xi21 11.03 Tf 8Td (290.646021)T)=

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1/2

F t(l r ~)= a

'

(ar) 2p(@+1)!
ar 121—&I + &
(ar) (46)

where a=2Z* jp and Z* is the effective nuclear
charge.
The two types of basis sets have very different spatial properties (e.g., casp behavior and localiza-tion), yet Fig. 3 shows that the energy levels of the t2 and a~ vacancy levels obtained with these basis functions agree to within 0.01 eV. Notice that we use the same number N of radial orbitals for each of the angular-momentum components of the wave function (I=1,2, 3,4 for tz and 1=0,3, 4 for a&).
This basis has therefore an enormous

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eludes the lowest nonspherical components even
though b, V(r) and bp(r) are nearly spherically
symmetric. The fact that only the first few

I com-

ponents of the wave function need to be retained in a Green's-function approach is illustrated in Table
VII. It illustrates the convergence of the energies and orbital-density localization parameters of the t2 and

a

~ vacancy levels with respect to the num-

ber of angular-momentum components L ",'„ in-cluded in the wave-function expansion of Eq. (28). If one restricts the wave-function representation to the single lowest

l component (i.e.

,

s orbitals for
the

a

&

states and
p orbitals for the t2 state), the re-
sulting

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This describes the three energy levels within a re-markable accuracy of 0.3% and correctly

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25.5

25.0

24.5

24.0

23.5

23.0

K
I I I I I I I I I

877 77 77 66 Q1 111111122 2 Q2
r
2.0

1.5

1.0

0.5

0.0

-0.5

FIG. 12. Quasiband structure for substitutional Cu in silicon. All the band-structure bands below 2 Ry are in-cluded. Five local quasibands, constructed from the

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0.04

0.

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)
Z
0
I-

ILI Q3 ~KI- D

LL

D

D

D

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2.

0

—

e Resonance

Q4—
t2 Gap State

1.

5

GM

1.0
Z
LU

0.

5

0OZ 00 0

I-0

Z'

—0.

5

UJ)~

— 1.0

~

— 1.

5

K

—2.

0

—~

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~

~

/ k=4 f x318

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~O~

W

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~ k=2

0.3—

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2

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Q.

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—ee

FIG. 17. Radial

1 components Gtt(

~

r

~

} [Eq. (29)] of

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500

400— CC
E
300

~oe Using Self Consistent Screening
Using Atomic Screening

L

C)

.c II)

200

100

0

aSO
~

& rooooOOOOOO ~ 0000000 ~ 000000000 ~ 000000
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&+

~ —100 O~
-200

ic guess b, V"(r)

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TABLE IX. Population analysis (in electrons) of the occupied states for the Si:Cu and the
silicon v:Cu

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I I) i I I I

0« —e Resonance (a)

0.06—

essentially passive, a simple, atomic view of this
impurity is likely to be wrong since extensive
charge redistribution and hybridization occurs in the s-p manifold.

0.04— VIII. COMPUTER TIME

0.02—

0.0
0.10

0.08—

I I I I I I I I

t2 Resonance

0.06—

~H II pp4-

s

0.02—

0.00—5 —4 —3 —2 —1 0 1 2 3 4 5
DISTANCE (a.u.)
FIG. 20. Radial densities of the Si:Cu e resonance in

the + (110) directions (a), and the sum of radial densi-ties for the three components of the t2 resonance, shown in the +(111)directions (b).

posite sign of the I =1 component in Si:Cu, but the same sign in the case of silicon vacancy (cf. Fig. 4). The gap state wave function in Si:Cu is hence distinctly different from the dangling-bond t2 wave function of the silicon vacancy.
The t2 and e resonances (Fig. 20) retain very much the overall characteristics of the atomic 3d orbital. Since the lobes of the e orbital point away from the nearest-neighbor ligands, this state is al-

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potential, 200 sec, and (iii) calculation of all over-lap integrals and quasibands entering the Green's function, 300 sec. (2) Iteration-dependent calcula-tions, given here per iteration, are (i) calculation of the potential perturbation from defect wave func-tion, 45 sec and (ii) the solution of the Green's-function problem, 110 sec. If we start from an atomic potential as an initial guess, the Jacobian update method requires seven iterations to con-verge to a few mRy accuracy. The calculations cost is hence 8.

6 min for the one-time expense,
plus 18 min

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X;(r)=B;;f;(r)+ Q BJP,(r),
j+i

(A4)

where the coefficients IB1]

are at this stage arbi-
trary. From Eqs. (Al), (A3), and (A4), one obtains the CFP that satisfies Eq. (A3) by construction, as:

g BPj(E(ej)P; (r)—
Va (E)

JAi

B(~f;(r)+ QB,J/J(r)
j+i

(A5)

Notice that any choice of [B;~I

in Eq. (A4) will
provide a solution to Eq. (A3) with the corrmt en-ergy E; However.,

the resulting wave function
X;(r) may not share the properties of the correct solution P; (r). Note further that with the CFP of Eq. (A5) one can solve Eq. (A3) even with a limit-ed basis set without fearing that the solution E; will converge to a low-lying ligandlike state ej,
which is the case in the standard

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=e'"'uj(k, r), (83)

where u~(k, r) is periodic with respect to transla-
tions by R&. It can therefore be Fourier-analyzed
as

R

=QF~(k, G)e'
G

and energies [ej9 (k)I

requires the diagonalization
of the host-crystal Hamiltonian Ho in the nonorthogonal basis of band-structure wave func-tions [P~ (k, r)J

and local Bloch functions

[XJ(k, r)) [Eq. (25)]. This then requires the evaluation of the matrix elements

(())j~ (k, r)~ 0 ~

(

k,

r

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unit cell. This poses no serious restriction since
the object of the quasiband approach is to have the
set [XJ(k, r) J

reproduce the localized parts of the
defect wave functions; the extended pieces of it are
then spanned by jPJ (k, r)J. Using this fact, one
obtains

&XJ(" r}l&0 IXJ(k r)&=&fj(r}l~o lfj'(r)& (89)

We now represent the local orbiter

r J. 27 the

k,are

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(r))Tj ET BT /Xi39 926 Tf0 794549 78.61 Td (.)Tj ET BT /Xi3 710.49 Tf6450.2491 2.01 Td(81089) k,

the

r

com (poand)Tj ET BT /Xi39 725 Tf 734446640.51 Tdiion paiocal

wa(is)Tj ET BT /Xi39 8.96 T139 83.46640.51 Tdahis

(k,)Tj ET BT /Xi392..41 Tf 5198946596.08 Td'XJ(k

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~o811 ())Tj ET BT /Xi390 2005 T5 8339.4 142611 Td(814 9) byto

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(k,)Tj ET BT /Xi39 18.44 Tf 86.1347 8.52 Td8((k,)Tj ET BT /Xi39261.6T Tf 103.4347 8816 Td (r))Tj ET BT /Xi39 12.57 Tf926.4347 2.01 Td~a(k,)Tj ET BT /Xi38 9.42 T1 137.43 143445 Td~

.813)ct, the isof by of the.

nent(is)Tj ET BT /Xi39 136 T3898777383 4.51 Tdiion +G) (.)Tj ET BT /Xi39 9.05 T451 9.8383 8.52 TdGivthen the is8889)1289) 84)ct,

one

the 812(r})Tj ET BT /Xi3908641 Tf1184533 274.73 Td (to)Tj ET BT /Xi39 8.45 T3 129413 274.73 Td (obtais)Tj ET BT /Xi39 136 T35674813 274.73 Tdahis

the

quasiband

wahe functio(r)Tj ET BT /Xi31011541 Tf11881329710.26 Td[Eq (.)Tj ET BT /Xi3 71.57 T33675.429712.61 Td (Bl)]is)Tj ET BT /Xi39 63.9 T3 9 7229651.21 Tdiband

the functiof isj89)

local

represeaiction

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S»——(g,(r) ~ 8(r) ~X,(k,r)}.

From Eqs. (27) and (B2) we obtain for the first matrix element in Eq. (C2),

Sq= QB&(k+G)e '"+o"Ki (k+G)i f Fzi(rj)i(~

i+Ger)8(r)r dr,
N o

0 P

(C3)

&(fg,*(r)8(r)fi(r RI)dr —. (C4)

Note that from this equation the advantage of in-troducing the cut-off function 8(r }becomes ap-parent: It reduces the number of two-center in-tegrals that need to be calculated.
The calculation of the integrals in Eq. (C4) in-volves the standard a-Lowdin expansion. How-ever, this technique has not been previously gen-eralized to include the treatment of arbitrary orbi-

where ~ is the displacement

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where the unitary matrix D' '

is the transformation matrix of spherical harmonics in the Condon-Shortley
phase convention under rotation of the Euler angles (a, b,c):
l

Yr (8,$)= g

D' ' (a,b, c)YI (O', P').
m'= —l

(Cl 1)

Furthermore, U'" is the unitary matrix relating spherical and Kubic harmonics of angular-quantum number
I:
l

KP (8,$}= g U'"pgYr (8,$).

m= —l

(C12)

The Euler angles (a,b, c) in Eqs. (C10) and (Cl 1) correspond to a rotation of the coordinate system at r =0 [the origin of the g,(r }functions] such that the polar axis (z axis) points along the vector R~. The explicit expression for the D matrices is

;~,;~,+

(—1)"[(l+m)!(l—m)!(1+m')!(l —m')!]' a!(1+m —a.)!(l—m

'—a)!(a+m' —m)!

'

2l —2z—m'+m ' 2sc+m' —m
b b
cos—
2

sin—
2

(C13)

where the summation over ~ includes all values

that make the arguments of the factorials non-
negative. Furthermore, Pr (x) are the associated
Legendre polynomials and kl are the spherical
harmonic normalization constants (in the Condon-Shortly phase convention):

Yr (8,$)=kr~PI (cos8)e', m &0

(8,$)=(—1) Yi '(8,$), m &0
'1/2 ' '

1/2

(1)~ 21+1 (1—m)!

4m (l+m)!

(C14)

In deriving these expressions, we have assumed that the coordinate system at r =R& is related to

the fixed coordinate system at r =0 through a translation by Rz (i.e.,

the two-coordinate systems
have the same orientation). Hence, their polar axes are parallel, but do not generally point along the direction of R~. The interpretation of the various factors in Eq. (CS) is then the following: The Q'- matrix elements to the right of the "transfer in-tegral" I first express the function fj(p } in Eq. (C5) at r =R~ in terms of spherical harmonics and then express this function in a rotated coordi-nate system whose polar axis is in the direction of Rz. Then the transfer integral I gives the resulting function in a rotated coordinate system at r =0, whose polar axis is also in the direction of Rz. This integral alone (without the & matrices) is the
only ingredient in the a-expansion technique de-
rived by Lowdin. Finally, the & matrix to the
left of the I gives the function in terms of spheri-

I

cal harmonics in a coordinate system rotated back to its original orientation and expresses this func-tion in terms of Kubic harmonics in that
the

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full BZ [Eq. (D2)] to sums over the irreducible BZ
(IBZ). The final results of this appendix are given
in Eqs. (D3), (D5), and (D8).
Since the expansion

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tion. In this appendix we derive explicit closed-form expressions for 5i(I

r I

) for Td defects in a
zinc-blende host crystal. The final results of this appendix are given in Eqs. (E16)—(E20), and (E26).

1. Charge density of the defected system

Using our expression (29) for the defect wave

functions f (r) in terms of local orbitals, we ob-
tain

8(r —R,)P (r)=QG; (I

r I

)E '

(r). (E2)
l

The charge density within the region defined by R, for spin o(o = T or g) is
occ da

pD(r)= X X X I e(r —R, V', (r
i,(o) a A,=l

needs to be valid only in the domain I

r I & I R, I,
much like in Eq. (E3). Since the host wave func-tions are often available as a Fourier series [c.f. Eq. (82)], one might construct from it a similar

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(E12)

We can make contact with the standard continuum Green s-function formalism by taking 8(r)=1, S=l. One then recognizes that the matrix elements B,b of Eq. (El 1) correspond to
EF

B.b = I—m J G'b(e)de,

where Eb is the Fermi energy and that PH(r) of Eq. (E10) corresponds to

PH(r)=2+g, (r

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This involves performing two simple one-dimensional radial integrals, exactly like in atomic calculations.
This procedure was tested successfully on a number of analytically solvable problems.

5. The change in the exchange-correlation potential

The exchange-correlation potential b V"'[pi),pH] is nonlinear with respect to pL) —pH [cf. Eq. (Sb)] and therefore cannot be evaluated from hp. Instead,

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the full energy scale with an energy mesh that can resolve any two roots. There exists however a very elegant algorithm, first used by Van der Avoird et al.,

6

for finding the roots of D (e) efficiently.
These authors considered the matrix

applied.

&roof. I.et aj(e) denote the eigenvectors of Q3(e):

Q3(e)a, (e)=p, (e)a,(e), (F6)

Q2(e) = V Go(e) V—V= —VQ i (e) (F2)

where V is a nonsingular matrix, and showed that the eigenvalues of Q2(e) always pass through zero with a negative slope, unless e equals one of the host-crystal energies ej(k). In this case, a number of eigenvalues [equal to the degeneracy of ei(k)] pass from —oo to + 00.
From these properties of the eigenvalues of Q2(e), it is clear that the number of roots n (ei, e2) of Eq. (Fl) in an energy interval [e&,ez] not con-taining a pole in the Green's function is given by

with the normalization requirement

aji(e)ai (e)=1. (F7)

Using the Hellmann-Feynman theorem, one gets that for all energies

PJ ~t()

dG (e)
aJ e
d

aJ e (FS)

Since the matrix dG (e)/de is symmetric, there ex-
ists some unitary matrix U(e) such that U(e)
)& [dG (e)/de] Ut(e) is diagonal. We get from Eq.
(FS) using the notation:

n (e&,e2)=n (e,)—n (e2), (F3) bj(e) = U(e)aj(e), (F9)
where n (e) denotes the number of positive eigen-
values of Q2(e). Thus, the energy roots of Eq.
(Fl) can be determined by repeated bisection of the
intervals until a desired accuracy is obtained.
To find the number of positive eigenvalues n (e)
of Q2 at some energy e, one can, of course, diago-
nalize Q2 directly, using standard techniques. A
much faster method, however, is to bring Qz into upper triangular form Qq by the Gauss elimination process and use the fact that the number of posi-tive eigenvalues of any real symmetric matrix 3 equals the number of positive diagonal elements in
AT.

In our applications, we have chosen to work
with the matrix

Q3(e)=GO(e) —V

'—=—Q|(e)V
rather than with Q2(e). The reason for this is that the construction of the matrix Q2(e) from the basic quantities Go(e) and V requires a double ma-trix multiplication VGO(e) V for each trial energy e=-e;. The computer time for performing these operations is much longer than inverting V once. Since Q3(e) is a symmetric matrix with only real eigenvalues, the equation detQ3(e) =0 has the same
roots as D (e)=0 since det V+ 0.
We now prove that the eigenvalues p,;(e) of Q3(e) obey the condition

dp;(e)
&0

that

d/l j

(e)

(F10)
We shall now show that the eigenvalues of
dG (e)/de (i.e.,

the diagonal elements in the ma-
trix U(e)[dG (e)/de]Ut(e)) are all nonpositive (the off-diagonal elements are, of course, zero). Consider a typical matrix element in the matrix dG (e)/de:

dG (e) p (aljk&(jk lp&

de i „[e—ej(k)]
After diagonalization we have

dG (e)-- o
hatt U()dG (

dE

yy

(+ l

J'k & (jk l && (F12)
[e—ej(k)]

(a l = U(e) (a l

lP&= lP&U"(e).

Thus, the eigenvalues of dG (e)/de are of the
form

for all energies different from the unperturbed one-electron energies, so that the method described

above for finding the roots of D(e)=0 can still be

dG (e)~

[e eJ~(k)]—(F14)

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by, Proc. Phys. Soc. London 90, 181 (1967);W. B.
Fowles, Phys. Status Solidi 26, 639 (1968). See, also,
discussion by A. M. Stoneham, in Theory of Defects in
Solids (Claredon, Oxford,