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APPENDIX A

DOUBLE-TIME GREEN FUNCTION.[89]

The double-time temperature dependent Green function was first introduced by Zubarev (1960). The principle definitions and basic equations of this techniques will be briefly reviewed.

Let X be any operator, then the grand canonical ensemble average is

$$X = Z^{-1}.\mathrm{Tr}\{X.\exp\left[-\beta.(H-\mu N)\right]\} \quad , \qquad \text{A1}$$

where

$$Z = \mathrm{Tr}\{\exp\left[-\beta.(H-\mu N)\right]\} . \qquad \text{A2}$$

Here H is the Hamiltonian, N is the total number operator, and

$$\beta = -1/kT$$

with k denoting the Boltzmann constant and T being the absolute temperature, and μ is the chemical potential.

Any operator A(t), in Heisenberg representation at time t, can be related to the operator A(O) at time O by

$$A(t) = e^{iHt}.A(O).e^{-iHt} , \qquad \text{A3}$$

The retarded (+) and advanced (-) Green function are defined by

$$<< A(t),B(t')>>^{(\pm)} = \pm i\Theta(\pm(t-t')).<[A(t),B(t')]_\eta>, \qquad A4$$

where
$$[A,B]_\eta = AB - \eta.BA \quad . \qquad A5$$

The value of η may be +1 or -1 depending on whether the statistics used is either Bose-Einstein or Fermi-Dirac. In A4 $\Theta(x)$ denotes the step function,

$$\Theta(x) = \begin{cases} 1 & x > 0 \\ 0 & x \leq 0 . \end{cases}$$

These Green functions can be shown to satisfy the equation of motion

$$\frac{id}{dt}<<A(t),B(t')>>^{(\pm)} = \delta(t-t').<[A(t),B(t')]_\eta>+<<\frac{id}{dt}A(t),B(t')>>^{(\pm)}$$

$$= (t-t').<[A(t),B(t')]_\eta>+<<[A(t),H(t)]_+ ,B(t')>>^{(\pm)} \qquad A6$$

At equilibrium, $<<A(t), B(t')>>^{(\pm)}$ are function of t-t' only. At this point we define the Fourier transform of the Green function, for real ω

$$<<A,B>>_\omega^{(\pm)} = (2\pi)^{-1}. \int_{-\infty}^{\infty} dt.<<A(t), B(t')>>.\exp(i\omega t) . \qquad A7$$

Zubarev (1960) showed that the Green function $<<A,B>>_\omega^{(\pm)}$ can be continued analytically in the complex ω plane. The function $<<A,B>>_\omega^{(\pm)}$ can thus be considered to be single analytical function in complex plane with a singularity on real axis. Thus we can omit the indice ± and simply write $<<A,B>>_\omega$ such that

$$<<A,B>>_\omega = \begin{cases} <<A,B>>_\omega^{(\pm)} & Im\omega>0 \\ <<A,B>>_\omega^{(-)} & Im\omega<0 \end{cases} \qquad A8$$

He also related the Green function to the correlation function $<B(t'), A(t)>$ as follow

$$<B(t'), A(t)> = i.\lim_{\varepsilon\to 0} \int_{\infty}^{\infty} d\omega . \left[<<A,B>>_{\omega+i\varepsilon} - <<A,B>>_{\omega-i\varepsilon} \right] . \exp\left[-\omega(t-t')\right] / \left\{ \exp\left[\beta(\omega-\mu)\right] - \eta \right\}. \qquad A9$$

Transforming A6 by A7 and using A8, we have

$$<<A,B>>_\omega = <\left[A,B\right]_\eta>/2\pi + <<\left[A,H\right]_+,B>>_\omega \qquad A10$$

The equation A6 and its corresponding Fourier transform, A10, represent the new Green function $<<\left[A,H\right]_+,B>>_\omega$. This Green function can be inserted into the equation of motion again, which gives the in new higher order Green function. Repeating, we get a chain of equation. We will need to take an approximation to close the chain. The appropreate approximation will depend on the problem being studied.

APPENDIX B

THE INTEGRAL PART OF THE SPIN σ ELECTRON'S OCCUPATION NUMBER n_σ

The Hartree-Fock approximation gives us the electron density distribution at the adatom shown in 5.2.4. Integrating this from the bottom of the band to Fermi level, we get the occupation number of spin σ electron contributed at the adatom if no localized states exist. If localized states exist, we just add the number of spin σ electron localized to the previous number (sec 5.2.7). The integral is

$$\mathfrak{J} = \int_{-1}^{x_F} dx . \frac{\pi^{-1} . 2 \lambda^2 \sqrt{1-x^2}}{(1-4\lambda^2).x^2 - 2(1-2\lambda^2).x_\sigma.x + x_\sigma^2 + 4\lambda^4} . \qquad \text{B1}$$

Defining

$$\Lambda = \pi^{-1}.2\lambda^2 \text{ , } a = 1-4\lambda^2, \text{ } b = -2(1-2\lambda^2).x_\sigma \text{ and } c = x_\sigma^2 + 4\lambda^4 \text{ ,} \qquad \text{B2}$$

we now can consider the following case :

<u>Case 1</u>, $a \neq 0$.

Letting $\alpha = c/a$ and $\beta = b/a$, B3

B1 becomes $\mathfrak{J} = A.(\mathcal{A} - \mathcal{B})$, B4 where

$$\mathcal{A} = \int_{-1}^{x_F} dx. \frac{1 + \alpha + \beta.x}{(\alpha + \beta.x + x^2)\sqrt{1-x^2}} \qquad \text{B.5.a}$$

and

$$\mathcal{B} = \int_{-1}^{x_F} dx. \frac{1}{\sqrt{1 - x^2}}$$

$$= \pi/2 + \arcsin x_F \; . \qquad \text{B5.b}$$

Case 1.1, $(1-2\lambda^2)^2 \neq x_\sigma^2$, $(1-2\lambda^2) \neq 0$, $x_\sigma \neq 0$.

Let us define $$x = B + \frac{t-1}{t+1}.D \; , \qquad \text{B6.a}$$

where $$B = \frac{(1-2\lambda^2)^2 + x_\sigma^2}{2(1-2\lambda^2).x_\sigma} \quad \text{and} \quad D = \frac{|(1-2\lambda^2)^2 - x_\sigma^2|}{2(1-2\lambda^2).x_\sigma} \qquad \text{B6.b}$$

Since $$1 + \alpha + \beta.B = 0 \quad \text{and} \quad B^2 - D^2 = 1 \; , \qquad \text{B7}$$

we find that

$$1 + \alpha + \beta.x = (1 + \alpha + \beta.B) + \beta.D.\frac{t-1}{t+1} = \beta.D.\frac{t-1}{t+1}, \qquad \text{B8}$$

$$\alpha + \beta.x + x^2 = (t+1)^{-2}.\left[(B^2 - 1 + \beta.D + 2.B.D + D^2).t^2 + 2.(B^2 - 1 - D^2).t + (B^2 - 1 - \beta.D - 2.B.D + D^2)\right]$$

$$= D.(t+1)^{-2}.\left[(\beta + 2(B+D)).t^2 - (\beta + 2(B-D))\right] \; , \qquad \text{B9}$$

$$1 - x^2 = 2D.(t+1)^{-2}.\left[(B-D) - (B+D).t^2\right] \qquad \text{B10}$$

and $$dx = 2D.(t+1)^{-2}.dt \; . \qquad \text{B11}$$

From B6.a, we obtain

$$t = -\frac{x - (B-D)}{x - (B+D)} \quad . \qquad B12$$

From B6.b, we can easily verify that B+D is never equal to zero so that B10 becomes

$$1 - x^2 = 2D.(B+D).(t+1)^{-2}.(|t_o| - t^2) \ . \quad B13$$

Case 1.1.1, $\beta + 2(B+D) \neq 0$.

We can rewriten B9 as

$$\alpha + \beta.x + x^2 = D.(\beta + 2(B+D)).(t+1)^{-2}.(t^2 + t_{-\frac{1}{2}\beta}). \qquad B14$$

Applying B14, 13, 11, 8 to B5.a, we get

$$\mathcal{A} = \frac{2\beta.D}{(\beta + 2(B+D)).\sqrt{2D.(B+D)}} . \int_{t_{-1}}^{t_F} dt. \frac{t-1}{(t^2 + t_{-\frac{1}{2}\beta}).\sqrt{|t_o| - t^2}} \quad .B15$$

Let us define $\mathcal{A} = E.(\mathcal{D} - \mathcal{E})$, B16

where $E = 2\beta.D.(\beta + 2(B+D)).(2D.(B+D))^{-\frac{1}{2}}$, B17

$$\mathcal{D} = \int_{t_{-1}}^{t_F} dt.t.(t^2 + t_{-\frac{1}{2}\beta})^{-1}.(|t_o| - t^2)^{-\frac{1}{2}} \quad B18.a$$

and

$$\mathcal{E} = \int_{t_{-1}}^{t_F} dt.(t^2 + t_{-\frac{1}{2}\beta})^{-1}.(|t_o| - t^2)^{-\frac{1}{2}} . \quad B18.b$$

B18.a can be evaluated by using the transformation

$$u = (|t_o| - t^2)^{-\frac{1}{2}} \quad . \tag{B19}$$

Then we get $\mathcal{D} = -\int_{u_{-1}}^{u_F} du.((|t_o| + t_{-\frac{1}{2}\beta}) - u^2)^{-1}$. B20

For $|t_o| + t_{-\frac{1}{2}\beta} = 0$, we have

$$\mathcal{D} = \int_{u_{-1}}^{u_F} du.u^{-2} = -u^{-1}\Big|_{u_{-1}}^{u_F} \quad . \tag{B21}$$

For $|t_o| + t_{-\frac{1}{2}\beta} \neq 0$, we can define

$$v = u.(||t_o| + t_{-\frac{1}{2}\beta}|)^{-\frac{1}{2}} \quad , \tag{B22}$$

By applying this into B20, we get the following results :

for $|t_o| + t_{-\frac{1}{2}\beta} > 0, \mathcal{D} = -\frac{1}{2}.(||t_o| + t_{-\frac{1}{2}\beta}|)^{-\frac{1}{2}}.\ln\left|\frac{1+v}{1-v}\right|\Big|_{v_{-1}}^{v_F}$. B23.a

for $|t_o| + t_{-\frac{1}{2}\beta} < 0, \mathcal{D} = (||t_o| + t_{-\frac{1}{2}\beta})^{\frac{1}{2}}.\arctan(v)\Big|_{v_{-1}}^{v_F}$. B23.b

From B18.b we can evaluate $\mathcal{E}$ by defining

$$\bar{u} = t.(|t_o| - t^2)^{-\frac{1}{2}} \quad . \tag{B24}$$

We then have $\mathcal{E} = \int_{\bar{u}_{-1}}^{\bar{u}_F} d\bar{u}.((|t_o| + t_{-\frac{1}{2}\beta}).\bar{u}^2 + t_{-\frac{1}{2}\beta})^{-1}$. B25

This integral can be integrated to give the following:

for $t_{-\frac{1}{2}\beta} = 0$, $\mathcal{E} = -((|t_o| + t_{-\frac{1}{2}\beta}).\bar{u})^{-1}\Big|_{\bar{u}_{-1}}^{\bar{u}_F}$, B26 for $t_{-\frac{1}{2}\beta} \neq 0$, $\varepsilon = t^{-1}_{-\frac{1}{2}\beta} \cdot \int_{\bar{u}_{-1}}^{\bar{u}_F} d\bar{u} \cdot \left[\left(\frac{|t_o| + t_{-\frac{1}{2}\beta}}{t_{-\frac{1}{2}\beta}} \right) \cdot \bar{u}^2 + 1 \right]^{-1}$. B27

If $(|t_o| + t_{-\frac{1}{2}\beta})/t_{-\frac{1}{2}\beta} = 0$, we get

$$\varepsilon = t^{-1}_{-\frac{1}{2}\beta} \cdot \bar{u} \Big|_{\bar{u}_{-1}}^{\bar{u}_F} . \qquad \text{B28}$$

If $(|t_o| + t_{-\frac{1}{2}\beta})/t_{-\frac{1}{2}\beta} \neq 0$, and we define

$$\bar{v} = \bar{u} \cdot \left[\frac{t_o + t_{-\frac{1}{2}\beta}}{t_{-\frac{1}{2}\beta}} \right]^{\frac{1}{2}} , \qquad \text{B29}$$

then we obtain the following results

for $(|t_o| + t_{-\frac{1}{2}\beta})/t_{-\frac{1}{2}\beta} > 0$,

$$\varepsilon = t^{-1}_{-\frac{1}{2}\beta} \cdot \left| \frac{|t_o| + t_{-\frac{1}{2}\beta}}{t_{-\frac{1}{2}\beta}} \right|^{-\frac{1}{2}} \cdot \arctan \bar{v} \Big|_{\bar{v}_{-1}}^{\bar{v}_F} \qquad \text{B30.a}$$

for $(|t_o| + t_{-\frac{1}{2}\beta})/t_{-\frac{1}{2}\beta} < 0$,

$$\varepsilon = \tfrac{1}{2} t^{-1}_{-\frac{1}{2}\beta} \cdot \left| \frac{|t_o| + t_{-\frac{1}{2}\beta}}{t_{-\frac{1}{2}\beta}} \right|^{-\frac{1}{2}} \cdot \ln \left| \frac{1+\bar{v}}{1-\bar{v}} \right| \Big|_{\bar{v}_{-1}}^{\bar{v}_F} . \qquad \text{B30.b}$$

Case 1.1.2, $\beta + 2(B+D) = 0$.

Equation B9 now becomes

$$\alpha + \beta.x + x^2 = -D.(\beta + 2(B-D)).(t+1)^{-2} \qquad \text{B31}$$

Applying B31, 13, 12, 11, 8 into B5 .a, we have

$$\mathcal{A} = \bar{E}.(\mathcal{T} - \xi) , \qquad \text{B32}$$

where
$$\bar{E} = 2\beta.D.(\beta + 2(B-D))^{-1}.(2D.(B+D))^{-\frac{1}{2}}, \qquad \text{B33}$$

$$\mathcal{T} = \int_{t_{-1}}^{t_F} dt.t.(|t_o| - t^2)^{-\frac{1}{2}} = -\frac{1}{2}.(|t_o| - t^2)^{\frac{1}{2}}\Big]_{t_{-1}}^{t_F} \qquad \text{B34.a}$$

$$\xi = \int_{t_{-1}}^{t_F} dt.(|t_o| - t^2)^{-\frac{1}{2}} = \arcsin(t./\sqrt{|t_o|})\Big]_{t_{-1}}^{t_F} \qquad \text{B34.b}$$

Case 1.2, $(1-2\lambda^2)^2 = x_\sigma^2 \neq 0$.

We find $\alpha + \beta.x + x^2 = (x - e_+).(x - e_-)$ B35

where $e_{\pm} = ((1-2\lambda^2).x_\sigma \pm 4\lambda^4)/(1-4\lambda^4)$. B36

If $1-2\lambda^2 = x_\sigma$, we have $e_+ (x_\sigma^2 + 4\lambda^4)/(x_\sigma^2 - 4\lambda^4)$, $e_- = 1$. B37.a

If $1-2\lambda^2 = -x_\sigma$, we get $e_+ = -1$, $e_- = -(x_\sigma^2 + 4\lambda^4)/(x_\sigma^2 - 4\lambda^4)$. B37.b

From B5.a we obtain

$$\mathcal{A} = \int_{-1}^{x_F} dx.\frac{1 + \alpha + \beta.x}{e_- + e_+} . \left[\frac{1}{x-e_+} - \frac{1}{x-e_+}\right] . (1-x^2)^{-\frac{1}{2}}$$

$$= K_+.\mathcal{R}_+ - K_-.\mathcal{R}_- , \qquad \text{B38}$$

where we have defined $K_{\pm} = (1 + \alpha + \beta . e_{\pm})/(e_{+} + e_{-})$ B39

and $$\mathcal{K}_{\pm} = \int_{-1}^{x_F} dx.(x-e_{\pm})^{-1}.(1 - x^2)^{-\frac{1}{2}} .$$ B40

By transforming $x = \cos\Theta$, and $\Theta = 2.\arctan u$, B41

we get $$\mathcal{K} = 2.e^{-1}.\int_{u_{-1}}^{u_F} du.\left[\left(\frac{2-e}{e}\right) - u^2\right]^{-1} ,$$ B42

where and e are understood to be subscribed + or − , corespondingly.

For $(2 - e)/e = 0$, $$\mathcal{K} = 2.(eu)^{-1}\Big|_{u_{-1}}^{u_F} .$$ B43

For $(2 - e)/e = 0$, let us first define

$$v = u.\left|\frac{2 - e}{e}\right|^{-\frac{1}{2}} ,$$ B44

so we get the following case.

For $(2 - e)/e > 0$, $$\mathcal{K} = e^{-1}.\left|\frac{2-e}{e}\right|^{-\frac{1}{2}} . \ln\left|\frac{1+v}{1-v}\right|\Bigg|_{v_{-1}}^{v_F} .$$ B45.a

For $(2 - e)/e < 0$, $$\mathcal{K} = -e^{-1} . \left|\frac{2-e}{e}\right|^{-\frac{1}{2}} . \arctan v\Big|_{v_{-1}}^{v_F} .$$ B45.b

Case 1.3, $1 - 2\lambda^2 = 0$.

From B2 and B3, for this case we have

$$A = \pi^{-1}, \quad \alpha = -(x_\sigma^2 + 1) , \quad \beta = 0 .$$ B46

The equation B5.a now becomes

$$\mathcal{A} = \int_{-1}^{x_F} dx.(1+\alpha).(x^2+\alpha)^{-1}.(1-x^2)^{-\frac{1}{2}}$$

$$= L.(\mathcal{L}_- - \mathcal{L}_+) \ , \qquad \text{B47}$$

where $$L = \frac{1}{2}.(|\alpha|)^{-\frac{1}{2}}.(1 + \alpha) \qquad \text{B48}$$

and $$\mathcal{L}_\pm = \int_{-1}^{x_F} dx.(x \pm \sqrt{|\alpha|})^{-1}.(1 - x^2)^{-\frac{1}{2}}. \qquad \text{B49}$$

By transfoming $x = \cos\Theta$, and $\Theta = 2.\arctan u$, B50

we get $$\mathcal{L}_\pm = 2.(|\alpha|)^{-\frac{1}{2}}. \int_{u_{-1}}^{u_F} du. \left[\frac{2 \pm \sqrt{|\alpha|}}{\sqrt{|\alpha|}} \pm u^2\right]^{-1} . \qquad \text{B51}$$

If $2 \pm \sqrt{|\alpha|} = 0$, $$\mathcal{L}_\pm = \mp 2.(|\alpha|)^{-\frac{1}{2}}.u^{-1}\Big]_{u_{-1}}^{u_F} . \qquad \text{B52}$$

If $2 \pm \sqrt{|\alpha|} \neq 0$, let us now define

$$v = u. \left|\frac{2 \pm \sqrt{|\alpha|}}{\sqrt{|\alpha|}}\right|^{\frac{1}{2}} , \qquad \text{B53}$$

so we get the following case.

for $2 \pm \sqrt{|\alpha|} > 0$, $$\mathcal{L}_+ = 2.(|2| + \sqrt{|\alpha|})^{-\frac{1}{2}} . \arctan v\Big]_{v_{-1}}^{v_F} \qquad \text{B54.a}$$

and $$\mathcal{L}_- = (|2| - \sqrt{|\alpha|})^{-\frac{1}{2}}.\ln\left|\frac{1+v}{1-v}\right|\Big]_{v_{-1}}^{v_F} . \qquad \text{B54.b}$$

for $2 \pm \sqrt{|\alpha|} < 0$, $\mathcal{L}_{+} = -(|2 + \sqrt{|\alpha|}|)^{-\frac{1}{2}} . \ln \left|\frac{1+v}{1-v}\right| \Big]_{v_{-1}}^{v_F}$ B55.a

and $\mathcal{L}_{-} = -2.(|2-\sqrt{|\alpha|}|)^{-\frac{1}{2}} . \arctan v \Big]_{v_{-1}}^{v_F}$. B55.b

Case 1.4, $x_{\sigma} = 0$.

The equation B3 becomes

$$\alpha = 4\lambda^4 . (1 - 4\lambda^2)^{-1} \text{ and } \beta = 0. \qquad \text{B56}$$

Similarly equation B5.a becomes

$$\mathcal{A} = \int_{-1}^{x_F} dx . (1 + \alpha) . (x^2 + \alpha) . (1 - x^2)^{-\frac{1}{2}} . \qquad \text{B57}$$

Defining $x = u.(1 - u^2)^{-\frac{1}{2}}$, B58

we have $\mathcal{A} = \frac{1+\alpha}{\alpha} \int_{u_{-1}}^{u_F} du . \left[\frac{1+\alpha}{\alpha} . u^2 + 1\right]^{-1}$ B59

If $\lambda > 0$, we have $\alpha > 0$ and also $(1 + \alpha)/\alpha > 0$, Thus

$$\mathcal{A} = \left|\frac{1-2\lambda^2}{2\lambda^2}\right| . \arctan \left|\frac{1-2\lambda^2}{2\lambda^2}\right| . u \Big]_{u_{-1}}^{u_F} . \qquad \text{B60}$$

Case 2, $a = 0$.

The equation B2 now becomes

$$A = (2\pi)^{-1}, \qquad b = -x_\sigma, \qquad c = x_\sigma^2 + 0.25. \qquad \text{B61}$$

while equation B1 can be written as

$$\mathcal{G} = (2\pi)^{-1} \cdot \int_{-1}^{x_F} dx \cdot (1 - x^2)^{\frac{1}{2}} \cdot (-x_\sigma \cdot x + x_\sigma^2 + 0.25)^{-1}. \qquad \text{B62}$$

Case 2.1, $x_\sigma = 0$.

The equation B62 now bexomes

$$\mathcal{G} = (2\pi)^{-1} \cdot \int_{-1}^{x_F} dx \cdot (1-x^2)^{\frac{1}{2}} / 0.25 .$$

$$= \frac{1}{2} + \pi^{-1} \cdot (\arcsin x_F + x_F \cdot \sqrt{1-x_F^2}) \qquad \text{B63}$$

Case 2.2, $x_\sigma \neq 0$.

In this case the equation B62 becomes

$$\mathcal{G} = -M \cdot \int_{-1}^{x_F} dx \cdot (1 - x^2)^{\frac{1}{2}} \cdot (x - f)^{-1}, \qquad \text{B64}$$

where $M = (2x_\sigma \cdot \pi)^{-1}$ and $f = (x_\sigma^2 + 0.25)/x_\sigma$. B65

Equation B64 can be writen as

$$\mathcal{G} = -M \cdot (-\text{[illegible]} - f \cdot \text{[illegible]} + (1-f^2) \cdot \text{[illegible]}), \qquad \text{B66}$$

where $\mathcal{M}$, $\mathcal{N}$ and $\mathcal{P}$ is defined as follows :

$$\mathcal{M} = \frac{1}{2}\cdot\sqrt{1-x_F^2} \ , \qquad \text{B67.a}$$

$$\mathcal{N} = \arctan x_F + \frac{1}{2} \qquad \text{B67.b}$$

and
$$\mathcal{P} = \int_{-1}^{x_F} dx.(1-x^2)^{\frac{1}{2}}.(x-f)^{-1} \ . \qquad \text{B67.c}$$

By transforming $x = \cos\Theta$, and $\Theta = 2.\arctan u$, B68

we get
$$= 2.f^{-1}.\int_{u_{-1}}^{u_F} du.\left[\frac{2-f}{f} - u^2\right]^{-1} \ . \qquad \text{B69}$$

Defining
$$v = u.\left|\frac{2-f}{f}\right|^{-\frac{1}{2}} \ , \qquad \text{B70}$$

we get the following case

for $(2-f)/f > 0$,
$$= f^{-1}.\left|\frac{2-f}{f}\right|^{-\frac{1}{2}}.\ln\left|\frac{1+v}{1-v}\right|\Bigg]_{v_{-1}}^{v_F} \ . \qquad \text{B71.a}$$

for $(2-f)/f < 0$,
$$= -2.f^{-1}.\left|\frac{2-f}{f}\right|^{-\frac{1}{2}}.\ \arctan v\Bigg|_{v_{-1}}^{v_F} \ . \qquad \text{B71.b}$$

APPENDIX C

THE SIMPLIFICATION OF Im $\left[Tr(G)\right]$.

Let us first define

$$I_{\mu\nu\eta}(E) = \int_0^\infty dt.\cos Et.J_\mu(t).J_\nu(t).J_\eta(t) , \quad C1$$

where the Bessel functions are given as follows

$$J_\eta(t) = \frac{(t/2)^\eta}{\Gamma(\eta+\frac{1}{2}).\Gamma(\frac{1}{2})} . \int_0^\pi d\Theta.\cos(t.\cos\Theta).\sin^{2\eta}\Theta, \quad C2$$

$$J_\mu(t).J_\nu(t) = \int_0^{\frac{\pi}{2}} d\phi.J_{\mu+\nu}(2t.\cos\phi).\cos(\mu-\nu)\phi , \quad C3$$

$$J_\mu(t).J_\nu(t).J_\eta(t) = \frac{1}{\Gamma(\eta+\frac{1}{2}).\Gamma(\frac{1}{2})} . \int_0^\pi d\Theta.\sin^{2\eta}\Theta. \int_0^{\frac{\pi}{2}} d\Theta.\cos(\mu-\nu)\phi .$$

$$.(\frac{t}{2})^\eta .\cos(t.\cos\Theta).J_{\mu+\nu}(2t.\cos\phi) . \quad C4$$

Substituting C4 into C1, we get

$$I_{\mu\nu\eta}(E) = \frac{1}{\Gamma(\eta+\frac{1}{2}).\Gamma(\frac{1}{2})} . \int_0^\pi d\Theta.\sin^{2\eta}\Theta. \int_0^{\frac{\pi}{2}} d\phi.\cos(\mu-\nu)\phi.$$

$$. \int_0^\infty dt.\cos Et.(\frac{t}{2})^\eta .\cos(t.\cos\Theta).J_{\mu+\nu}(2t.\cos\phi)$$

$$= \frac{1}{\Gamma\ \eta+\frac{1}{2}).\Gamma(\frac{1}{2})} \int_0^\pi d\Theta.\sin^2\Theta. \int_0^{\frac{\pi}{2}} d\phi.\cos(\mu-\nu)\phi .$$

$$M_{\mu\nu\eta}(E,\Theta,\phi) , \quad C5$$

where we have define

$$M_{\mu\nu\eta}(E,\theta,\emptyset) = \int_0^\infty dt.\cos Et.(\frac{t}{2})^\eta .\cos(t.\cos\theta).J_{\mu+\nu}(2t.\cos\theta). \quad C6$$

Equation C6 can be rewriten as

$$M_{\mu\nu\eta}(E,\theta,\emptyset) = \int_0^\infty dt.\frac{1}{2}(\cos(E-\cos\theta)t + \cos(E+\cos\theta)t).(\frac{t}{2})^\eta .$$

$$. J_{\mu+\nu}(2t.\cos\emptyset)$$

$$= \frac{1}{2}(M^-_{\mu\nu\eta}(E,\theta,\emptyset) + M^+_{\mu\nu\eta}(E,\theta,\emptyset)), \quad C7$$

where we **have defined**

$$M^{\pm}_{\mu\nu\eta}(E,\theta,\emptyset) = \int_0^\infty dt.\cos(E\pm\cos\theta)t.(\frac{t}{2})^\eta J_{\mu+\nu}(2t.\cos\emptyset). \quad C8$$

For $(\mu,\nu,\eta) = (0,0,0)$, we have

$$M^{\pm}_0(E,\theta,\emptyset) = \int_0^\infty dt.\cos(E\pm\cos\theta)t.J_0(2t.\cos\emptyset). \quad C9$$

Puting C9 into C5, for $(\mu,\nu,\eta,) = (0,0,0)$, we get

$$I_0(E) = \frac{1}{2}.\pi^{-2}.(I^-_0(E) + I^+_0(E)), \quad C10$$

where $$I^{\pm}_0(E) = \int_0^\pi d\theta. \int_0^{\frac{\pi}{2}} d\emptyset.M^{\pm}_0(E,\theta,\emptyset) . \quad C11$$

From the table of intergral

$$M^{\pm}_0(E,\theta,\emptyset) = \begin{cases} ((2\cos\emptyset)^2 - (E\pm\cos\theta)^2)^{-\frac{1}{2}} & ; 0 < E\pm\cos\theta < 2\cos\emptyset , \\ \infty & ; E\pm\cos\theta = 2\cos\emptyset, \\ 0 & ; 0 < 2\cos\emptyset < E\pm\cos\theta . \end{cases} \quad C12$$

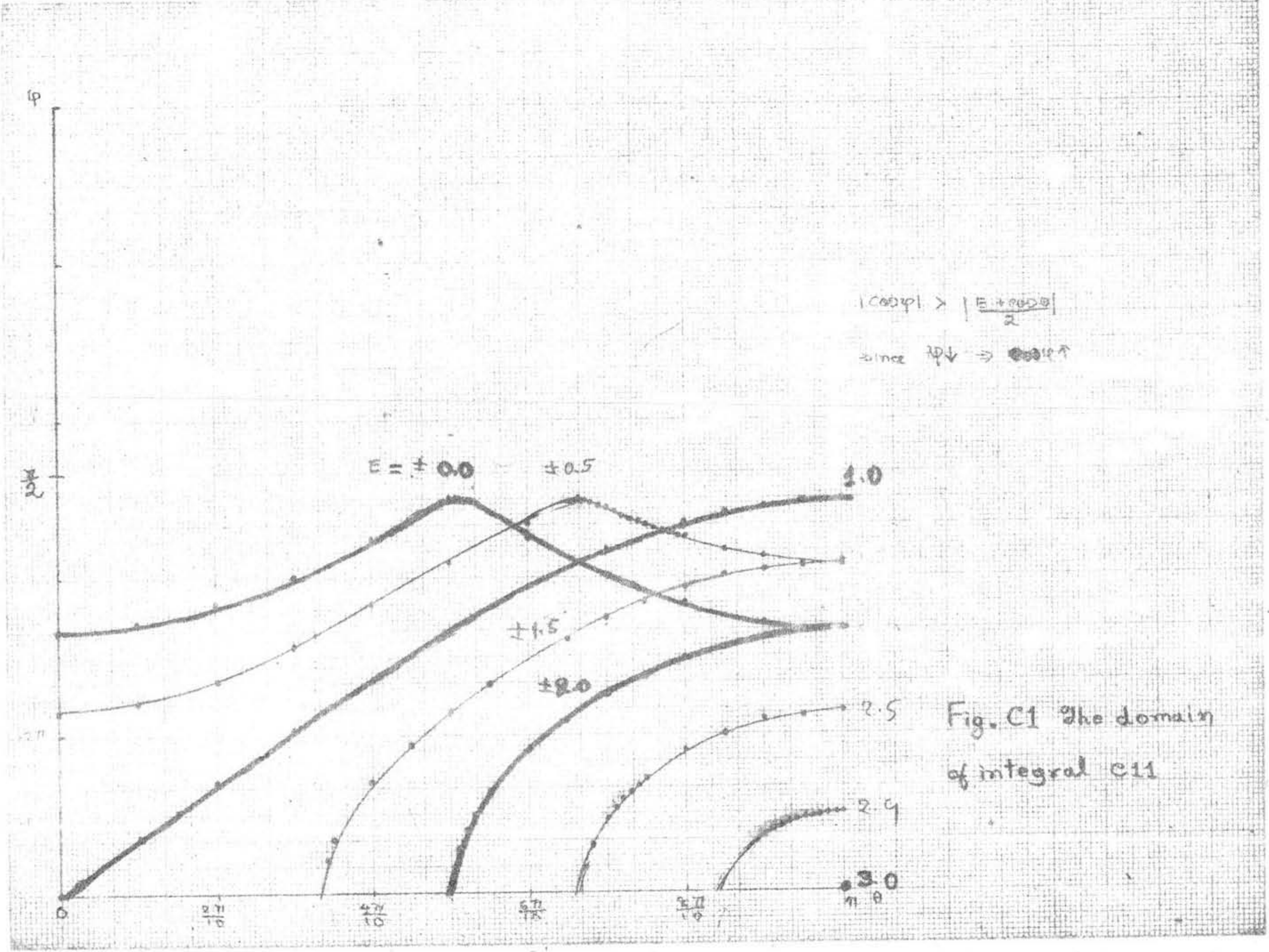


Fig. C1 The domain of integral C11

Let us consider the domain of integration C11. From C12, we find the following results.

If $|E| \leq 1$, we have $0 \leq \theta \leq \pi$ while $0 \leq \phi \leq \cos^{-1}(|E \pm \cos\theta|/2)$.

If $|E| > 1$, we have $\cos^{-1}(2-E) \leq \theta \leq \pi$ while $0 \leq \phi \leq \cos^{-1}(E+\cos\theta/2)$

or $0 \leq \theta \leq \cos^{-1}(E-2)$ while $0 \leq \phi \leq \cos^{-1}(E-\cos\theta/2)$.

This has shown graphically in Fig. C1. Since the integral is known to be symmetric with respect to E (see C6, it contain only cosEt that depend on E), we need to work only for E≥0. Putting C12 into C11 and applying the domain of integral discussed above, we have

$$I_{\circ}^{\pm}(E) = \int_{\circ}^{\cos^{-1}(|E\pm\cos\theta|/2)} d\theta d\phi \left[(2\cos\phi)^2-(E\pm\cos\theta)^2\right]^{-\frac{1}{2}}$$

$$\text{or } = \int_{0}^{\cos^{-1}(E\pm\cos\theta/2)} d\theta d\phi \cdot \left[\left[1-(E\pm\cos\theta/2)^2\right] \cdot \left[1-\frac{\sin^2\phi}{1-(E\pm\cos\theta/2)^2}\right]\right]^{-\frac{1}{2}} \cdot \quad C13$$

Defining $\sin u = \sin\phi . [(1-E\pm\cos\theta)^2/4]^{-\frac{1}{2}}$, C14

then we have $d\phi = (1-(E\pm\cos\theta)^2/4)^{-\frac{1}{2}} \cdot \frac{\cos u . du}{\cos\phi}$. C15

From C14, it is easily find that

$$u = \arcsin\left[(1-\cos^2\phi)^{-\frac{1}{2}} . (1-(E\pm\cos\theta)^2/4^{-\frac{1}{2}}\right] . \quad C16$$

Applying C14, 15, 16 into C13, we get

$$I_{\circ}^{\pm}(E) = \int_{\circ}^{\frac{\pi}{2}} d\theta du . \left[1-(1-(E\pm\cos\theta)^2/4).\sin^2 u\right]^{-\frac{1}{2}} . \quad C17$$

The integration over u gives the complete elliptic integral K9k), where k is a function of θ defined by,

$$k^2 = 1 - (E \pm \cos\theta)^2/4 \qquad C18$$

The integral C17 then can be rewriten as

$$I_o^{\pm}(E) = \int_{\theta_1}^{\theta_2} d\theta . K(\sqrt{1-(E \pm \cos\theta)^2/4}), \qquad C19$$

where θ_1 and θ_2 are the lower and upper bound of the integral domain, discussed previously (see Fig.C1 also).

Appendix D

MATRIX REPRESENTATION FOR IMPURITY PROBLEM.

In this appendix we will study the special properties of the matrix representation of the impurity problem. Usually we use the state vectors $|\ell\sigma\rangle$ and $|k\sigma\rangle$ of the isolated, unperturbed, systems as basis. So that the matrix representation of any operators $\hat{M}$ can be writen in block form as

$$M_{\sigma} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} , \qquad \text{D1}$$

where

$$\left.\begin{aligned} & M_{11} = \left[\langle\ell\sigma|\hat{M}|\ell\sigma\rangle\right] , \quad M_{12} = \left[\langle\ell\sigma|\hat{M}|k_1\sigma\rangle , \langle\ell\sigma|\hat{M}|k_2\sigma\rangle , \; . \; . \; .\right] \\ & M_{21} = \begin{bmatrix} \langle k_1\sigma|\hat{M}|\ell\sigma\rangle \\ \langle k_2\sigma|\hat{M}|\ell\sigma\rangle \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} , M_{22} = \begin{bmatrix} \langle k_1\sigma|\hat{M}|k_1\sigma\rangle , \langle k_1\sigma|\hat{M}|k_2\sigma\rangle & \cdots \\ \langle k_2\sigma|\hat{M}|k_1\sigma\rangle , \langle k_2\sigma|\hat{M}|k_2\sigma\rangle & \cdots \\ \cdot & \cdots \\ \cdot & \cdots \\ \cdot & \cdots \end{bmatrix} \end{aligned}\right\} . \qquad \text{D2}$$

Let us define

$$M_\sigma(1) = \begin{bmatrix} M_{11} & O_{12} \\ O_{21} & M_{22} \end{bmatrix}, \; M_\sigma(2) = \begin{bmatrix} O_{11} & M_{12} \\ M_{21} & O_{22} \end{bmatrix}, \; M_\sigma(3) = \begin{bmatrix} M_{11} & M_{12} \\ O_{21} & O_{22} \end{bmatrix}, \; M_\sigma(4) = \begin{bmatrix} O_{11} & O_{12} \\ M_{21} & M_{22} \end{bmatrix}$$

and

$$M_\sigma(5) = \begin{bmatrix} M_{11} & O_{12} \\ O_{21} & O_{22} \end{bmatrix} \qquad \text{D3}$$

From this simple projected matrix, all matrix of the problem can be formulated. The multiplication of these matrices gives us the special properties (which we use in chapter V), i.e.

$$A_\sigma(1).A_\sigma(1) = B_\sigma(1) \; ; \quad A_\sigma(2).A_\sigma(2) = C_\sigma(1) \; ;$$

$$A_\sigma(1).A_\sigma(2) = D_\sigma(2) \; ; \quad A_\sigma(2).A_\sigma(1) = E_\sigma(2) \; .$$

The type II projection have very interesting properties in that all matrix function of type II matrix can be expressed as

$$F\left[M_\sigma(2)\right] = a.I_\sigma + b.M_\sigma(2) + c.M_\sigma(2)^2, \qquad \text{D4}$$

where I_σ is unit matrix, and a, b, c are scalar quantities.

If we normalize $M_\sigma(2)$ by $\sqrt{M_{12}\,M_{21}}$, which is scalar quantity, we find that

$$\bar{M}_\sigma(2)^{2m-1} = \bar{M}_\sigma(2) \qquad \text{D5.a}$$

and

$$\bar{M}_\sigma(2)^{2m} = \bar{M}_\sigma(2).\bar{M}_\sigma(2) = \bar{M}_\sigma(2)^2. \qquad \text{D5.b}$$

This prove the statement given in D4.

Appendix E

BS-DECOUPLING SCHEME[96]

BS use the Hubbard decoupling technique to define[92]

$$n^{\alpha}_{\ell\sigma} = \begin{cases} n_{\ell\sigma} & \alpha = + \\ 1 - n_{\ell\sigma} & \alpha = - \end{cases} \quad \text{E1}$$

Defining $$c^{\alpha}_{\ell\sigma} = c_{\ell\sigma} n^{\alpha}_{\ell\bar{\sigma}} \quad \text{E2}$$

and $$\varepsilon_{\alpha} = \varepsilon_{\ell} + \delta_{\alpha +} U , \quad \text{E3}$$

we have $$n^{\alpha}_{\ell\sigma} n^{\beta}_{\ell\sigma} = \delta_{\alpha\beta} \cdot n^{\alpha}_{\ell\sigma} , \quad \text{E4}$$

$$\left.\begin{aligned} &[c^{\alpha}_{\ell\sigma}, c^{+}_{k\sigma'}] = 0 , \quad [c^{\alpha}_{\ell\sigma}, c_{\ell\sigma'}] = \alpha \cdot c_{\ell\sigma} c_{\ell\bar{\sigma}} \cdot \delta_{\bar{\sigma}\sigma'} , \\ &[c^{\alpha}_{\ell\sigma}, c^{+}_{\ell\sigma'}] = n^{\alpha}_{\ell\bar{\sigma}} \cdot \delta_{\sigma\sigma'} - \alpha \cdot c^{+}_{\ell\bar{\sigma}} c_{\ell\sigma} \cdot \delta_{\sigma\sigma} , \\ &[c^{\alpha}_{\ell\sigma}, n_{\ell\sigma'}] = c^{\alpha}_{\ell\sigma} \cdot \delta_{\sigma\sigma'} \quad \text{and} \quad [c^{\alpha}_{\ell\sigma}, n_{\ell\sigma'} n_{\ell\bar{\sigma}'}] = 2c^{\alpha}_{\ell\sigma} \cdot \delta_{\alpha +} \cdot \delta_{\sigma\sigma'} \cdot \end{aligned}\right\} \quad \text{E5}$$

Defining $$G_{\alpha\beta}(\omega) = \langle\langle c^{\alpha}_{\ell\sigma}, c^{\beta +}_{\ell\sigma} \rangle\rangle , \quad \text{E6}$$

and retting $V_{\ell k} = 0$, we have

$$\omega \cdot G^{0}_{\alpha\beta} = \langle n^{\alpha}_{\ell\bar{\sigma}} \rangle \cdot \delta_{\alpha\beta}/2\pi + \varepsilon_{\ell} \cdot G^{0}_{\alpha\beta} + U \cdot G^{0}_{\alpha\beta} \cdot \delta_{\alpha +}$$

or $$G^{0}_{\alpha\beta} = \frac{\langle n^{\alpha}_{\ell\bar{\sigma}} \rangle \cdot \delta_{\alpha\beta}}{2\pi \cdot (\omega - \varepsilon_{\alpha})} \quad \text{E7}$$

Defining $$X = \begin{pmatrix} x_{--} & x_{-+} \\ x_{+-} & x_{++} \end{pmatrix} ,$$ E8

we can write E7 explicitly as

$$G^{o} = \frac{1}{2\pi} \circ \begin{pmatrix} n_{\bar{\sigma}}^{-}/(\omega-\varepsilon_{-}) & 0 \\ 0 & n_{\bar{\sigma}}^{+}/(\omega-\varepsilon_{+}) \end{pmatrix} .$$ E9

Defining $$\Lambda = \frac{1}{2\pi} \circ \begin{pmatrix} n_{\bar{\sigma}}^{-} & 0 \\ 0 & n_{\bar{\sigma}}^{+} \end{pmatrix} ,$$ E10

then we have $$G^{o}_{\ell\ell\sigma}(\omega) = \sum_{\alpha\beta} G^{o}_{\alpha\beta}(\omega) = \frac{1}{2\pi} \circ \left[\frac{1-n_{\bar{\sigma}}}{\omega - \varepsilon_{\ell}} + \frac{n_{\bar{\sigma}}}{\omega - \varepsilon_{\ell} - U} \right] ,$$ E11

which is equivalent to 5.3.6.a.

BS suggested the self-energy matrix equation of the form

$$G = G^{o} + G^{o} \circ M \circ G ,$$ E12

where M is the self-energy matrix to be used. Note that G and G^{o} matrix representations of the Green function are not exactly single particle Green functions. In fact E12 has the two particle correlation as shadow. The interpretution of two propagators, which has been discussed in chapter IV, are G^{o}_{--} and G^{o}_{++} in the zero coupling limit. When the coupling $V_{k\ell}$ is considered, the two propagators are the fundamental propagators of the spin σ electron propagator $G^{\sigma}_{\ell\ell}$. For $V_{\ell k} \neq 0$, we have

$$(\omega - \varepsilon_{\alpha}) \circ G_{\alpha\beta} = \langle n^{\alpha}_{\ell\bar{\sigma}} \rangle \circ \delta_{\alpha\beta}/2\pi + \langle\langle d^{\alpha}_{\ell\sigma}, c^{\beta+}_{\ell\sigma} \rangle\rangle ,$$ E13

where $$d^{\alpha}_{\ell\sigma} = \sum_k \cdot \left[V_{\ell k} \cdot n^{\alpha}_{\ell\bar{\sigma}} c_{k\sigma} + \alpha \cdot (V_{\ell k} \cdot c^{\dagger}_{\ell\bar{\sigma}} c_{k\bar{\sigma}} c_{\ell\sigma} - V_{k\ell} \cdot c^{\dagger}_{k\bar{\sigma}} c_{\ell\bar{\sigma}} c_{\ell\sigma}) \right] \quad \text{E14.a}$$

$$= d^{\alpha 1}_{\ell\sigma} + \alpha \cdot (d^{2}_{\ell\sigma} - d^{3}_{\ell\sigma}) \ . \quad \text{E14.b}$$

The equation of motion for the second term on the right of equation E13 is

$$\langle\langle d^{\alpha}_{\ell\sigma}, c^{\beta +}_{\ell\sigma} \rangle\rangle \cdot (\omega - \varepsilon_{\beta}) = \langle \{ d^{\alpha}_{\ell\sigma}, c^{\beta +}_{\ell\sigma} \} \rangle \ /2\pi + \langle\langle d^{\alpha}_{\ell\sigma}, d^{\beta}_{\ell\sigma} \rangle\rangle \ . \quad \text{E15}$$

Defining

$$B_{\alpha\beta} = \langle \{ d^{\alpha}_{\ell\sigma}, c^{\beta\dagger}_{\ell\sigma} \} \rangle /2 \ . \quad \text{E16}$$

and $$D_{\alpha\beta} = \langle\langle d^{\alpha}_{\ell\sigma}, d^{\beta\dagger}_{\ell\sigma} \rangle\rangle \quad \text{E17}$$

we see that when E15 substituted into E13, the new matrix equation is

$$(A^{-1} \cdot G^{\circ})^{-1} \cdot G = A + (B + D) \cdot (A^{-1} \cdot G^{\circ}) \ .$$

From E12, we can find the formal solution of the Green function, Applying this into the equation, we have

$$(A^{-1} \cdot G^{\circ})^{-1} \cdot (I - G^{\circ} \cdot M)^{-1} \cdot G^{\circ} = A + (B + D) \cdot (A^{-1} \cdot G^{\circ}),$$

or $$(A^{-1} \cdot G^{\circ})^{-1} \cdot (I - G^{\circ} \cdot M)^{-1} = (A^{-1} \cdot G^{\circ})^{-1} + (B + D) \cdot A^{-1} .$$

Rearranging the first term on the right hund ride of the equation, we have

$$(A^{-1} \cdot G^{\circ})^{-1} \cdot G^{\circ} \cdot M \cdot (I - G^{\circ} \cdot M)^{-1} = (B + D) \cdot A^{-1} \ .$$

Multiplying the above equation by A, we get

$$A.M.(I - G^{0}.M)^{-1}.A = B + D. \qquad \text{E18}$$

Now, the problem is to find B and D. From E16, we have

$$\{d^{\alpha 1}_{\ell\sigma}, c^{\beta\dagger}_{\ell\sigma}\} = \sum_k V_{\ell k}.(\delta_{\alpha\beta}.n^{\alpha}_{\ell\sigma}.\{c_{k\sigma}, c^{\dagger}_{\ell\sigma}\}) = 0 ,$$

and

$$\{d^{2}_{\ell\sigma}, c^{\beta\dagger}_{\ell\sigma}\} = \sum_k V_{\ell k}.(c^{\dagger}_{\ell\bar\sigma} c_{k\bar\sigma} n^{\beta}_{\ell\sigma} + [n^{\beta}_{\ell\bar\sigma}, c^{\dagger}_{\ell\bar\sigma} c_{k\bar\sigma}].n_{\ell\sigma})$$

$$= \sum_k V_{\ell k}.c^{\dagger}_{\ell\bar\sigma} c_{k\bar\sigma}.(n^{\beta}_{\ell\bar\sigma} + \beta.n_{\ell\sigma}) .$$

Similarly, we have

$$\{d^{3}_{\ell\sigma}, c^{\beta\dagger}_{\ell\sigma}\} = \sum_k V_{k\ell}.c^{\dagger}_{k\bar\sigma} c_{\ell\bar\sigma}.(n^{\beta}_{\ell\bar\sigma} - \beta.n_{\ell\sigma}) .$$

Since $\langle c^{\dagger}_{\ell\bar\sigma} c_{k\bar\sigma}\rangle = \langle c^{\dagger}_{k\bar\sigma} c_{\ell\bar\sigma}\rangle$, we have

$$B_{\alpha\beta} = \frac{\alpha\beta}{2\pi}.\sum_k (V_{\ell k}.\langle c^{\dagger}_{k\bar\sigma} c_{\ell\bar\sigma} n_{\ell\sigma}\rangle + V_{k\ell}.\langle c^{\dagger}_{\ell\bar\sigma} c_{k\bar\sigma} n_{\ell\sigma}\rangle) . \qquad \text{E19}$$

We now need to obtain the Green function $\langle\langle c_{\ell\bar\sigma} n_{\ell\sigma}, c_{k\bar\sigma}\rangle\rangle$ and its conjugate. BS suggested that

$$B_{\alpha\beta} = \frac{\alpha\beta.q}{2\pi} , \qquad \text{E20}$$

with q being treated differently in weak and strong case. Their work is not self- consistent with $n_{\ell k}$, $n_{k\ell}$ and $n_{kk'}$ since they truncated the Green function $\langle\langle c_{\ell\bar\sigma} n_{\ell\sigma}, c^{\dagger}_{k\sigma}\rangle\rangle$ at first order of $V_{\ell k}$. From the definition E14 and E17, we have

$$D_{\alpha\beta} = \langle\langle d^{\alpha 1}_{\ell\sigma}, d^{\beta 1^+}_{\ell\sigma} + \alpha.(\langle\langle d^{2}_{\ell\sigma}, d^{\beta 1^+}_{\ell\sigma}\rangle\rangle - \langle\langle d^{3}_{\ell\sigma}, {}^{\beta 1^+}_{\ell\sigma}\rangle\rangle$$

$$\beta.(\langle\langle d^{\alpha 1}_{\ell\sigma}, d^{2^+}_{\ell\sigma}\rangle\rangle - \langle\langle d^{\alpha 1}_{\ell\sigma}, d^{3^+}_{\ell\sigma}\rangle\rangle) + \alpha\beta.(\langle\langle d^{2}_{\ell\sigma}, d^{2^+}_{\ell\sigma}\rangle\rangle$$

$$- \langle\langle d^{2}_{\ell\sigma}, d^{3^+}_{\ell\sigma}\rangle\rangle - \langle\langle d^{3}_{\ell\sigma}, d^{2^+}_{\ell\sigma}\rangle\rangle + \langle\langle d^{3}_{\ell\sigma}, d^{3^+}_{\ell\sigma}\rangle\rangle). \qquad \text{E21}$$

They developed the equation of motion for all Green function in E21 only up to zero order in $V_{\ell k}$. The result is

$$D_{\alpha\beta} = \frac{\langle n^{\alpha}_{\ell\bar{\sigma}}\rangle . \delta_{\ell\sigma}}{2\pi} . \Sigma_{o} + \frac{\alpha\beta . \gamma . \Sigma_{o}}{2\pi} , \qquad \text{E22}$$

where γ denoting the weak and strong coupling case and having the values $\frac{1}{2}$ and 2, respectively. We can write

$$\Lambda.M.\Lambda. = \Lambda.\Sigma_{o} + C.m , \qquad \text{E23}$$

where $$C_{\alpha\beta} = \alpha\beta/2\pi \qquad \text{E24}$$

and $$m = \gamma.\Sigma_{o} + q \qquad \text{E25}$$

Substituting E23 into E12, we get

$$G = \left[I - G^{o}.(\Lambda^{-1}.\Sigma_{o} + \Lambda^{-1}.C.\Lambda^{-1}).m\right]^{-1} .G^{o}. \qquad \text{E26}$$

Defining $C = (I + J)/2\pi$ and $J = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$, where the J matrix has similar properties as the type II matrix defined in Appendix D, i.e. $J^2 = I$; and defining

$$\bar{G} = \left[I - G^{\circ}.A^{-1}.(\Sigma_{o}.I + \frac{m}{2\pi}.A^{-1})\right]^{-1}.G^{\circ}.A^{-1} \qquad \text{E27.a}$$

$$= \begin{pmatrix} \dfrac{2\pi.g}{1-2\pi.g.(\Sigma_{o}+m/n^{-1})} & 0 \\ 0 & \dfrac{2\pi.g'}{1-2\pi.g'.(\Sigma_{o}+m/n^{+})} \end{pmatrix} \qquad \text{E27.b}$$

where $g = G^{\circ}_{--}/n^{-}$ and $g' = G^{\circ}_{++}/n^{+}$;

and also defining

$$Z = \frac{m}{2\pi}.\bar{G}.J.A^{-1}$$

$$\begin{pmatrix} 0 & \dfrac{-2\pi.g.m/n^{+}}{1-2\pi.g.(\Sigma_{o}+m/n^{-1})} \\ \dfrac{-2\pi.g'.m/n^{-}}{1-2\pi.g'.(\Sigma_{o}+m/n^{-})} & 0 \end{pmatrix}.$$

E26 becomes

$$G = (I - Z)^{-1}.\bar{G}.A$$

$$= I + \frac{Z+Z^{2}}{1+\det(Z)}.\bar{G}.A$$

$$= \frac{I+Z}{1+\det(Z)}.\bar{G}.A \qquad \text{E28}$$

$$= \frac{1}{1+\det(Z)}. \begin{bmatrix} \dfrac{2\pi.g.n^{-}}{1-2\pi.g.(\Sigma_{o}+m/n^{-})} & \det(Z).n^{-}.n^{+}/m \\ \det(Z).n^{-}.n^{+}/m & \dfrac{2\pi.g'.n^{+}}{1-2\pi.g'.(\Sigma_{o}+m/n^{+})} \end{bmatrix} \qquad \text{.E29}$$

since

$$G^{\sigma}_{\ell\ell}(\omega) = \Sigma_{\alpha\beta} \cdot G_{\alpha\beta}(\omega) \quad ,$$

we get

$$G^{\sigma}_{\ell\ell}(\omega) = \frac{1}{1+\det(Z)} \cdot \left[\frac{2\pi \cdot g \cdot n^-}{1-2\pi \cdot g \cdot (\Sigma_o + m/n^-)} + \frac{2\pi \cdot g' \cdot n^+}{1-2\pi \cdot g' \cdot (\Sigma_o + m/n^+)} + 2\det(Z) \cdot n^- \cdot n^+/m \right]$$

$$= \frac{2\pi \cdot g \cdot n^- \cdot \left[1-2\pi \cdot g' \cdot (\Sigma_o + m/n^+)\right] + 2\pi \cdot g' \cdot n^+ \cdot \left[1-2\pi \cdot g \cdot (\Sigma_o + m/n^{-1})\right] - 2(2\pi)^2 \cdot g \cdot g' \cdot m}{\left[1-2\pi \cdot g' \cdot (\Sigma_o + m/n^+)\right] \cdot \left[1-2\pi \cdot g \cdot (\Sigma_o + m/n^{-1})\right] - (2\pi)^2 \cdot g \cdot g' \cdot m^2/(n^- \cdot n^+)}$$

$$= \frac{\left[2\pi \cdot g \cdot (1-2\pi \cdot g' \cdot \Sigma_o) \cdot n^-\right] + \left[2\pi \cdot g' \cdot (1-2\pi \cdot g \cdot \Sigma_o) \cdot n^+\right] \frac{(2\pi)^2 \cdot g \cdot g' \cdot m \cdot (n^{-2} + 2n^- \cdot n^+ + n^{+2}}{n^- \cdot n^+}}{\left[(1-2\pi \cdot g' \cdot \Sigma_o) - 2\pi \cdot m \cdot g'/n^+\right] \cdot \left[(1-2\pi \cdot g \cdot \Sigma_o) - 2\pi \cdot m \cdot g/n^-\right] - (2\pi)^2 \cdot g \cdot g' \cdot m^2/(n^- \cdot n^+)}$$

$$= \frac{n^- \cdot n^+ \cdot \left[(\omega - \varepsilon_+ - \Sigma_o) \cdot n^- + (\omega - \varepsilon_- - \Sigma_o) \cdot n^+\right] - m}{\left[(\omega - \varepsilon_+ - \Sigma_o) \cdot n^+ - m\right] \cdot \left[(\omega - \varepsilon_- - \Sigma_o) \cdot n^- - m\right] - m^2} \quad . \qquad \text{E31}$$

$$\Gamma^{\ell\ell}_{\ell\ell\sigma}(\omega) = \underset{\beta}{\Sigma} \cdot G_{+\beta}(\omega) \quad ,$$

we get

$$\Gamma^{\ell\ell}_{\ell\ell\sigma}(\omega) = \frac{1}{1+\det(Z)} \cdot \left[\frac{\det(Z) \cdot n^- \cdot n^+}{m} + \frac{2\pi \cdot g' \cdot n^+}{1-2\pi \cdot g' \cdot (\Sigma_o + m/n^+)} \right] \cdot \qquad \text{E32}$$

The same result can be solved from the formal equation E12 if we know M. From E23, we find that

$$M = A^{-1} \cdot \Sigma_o + m \cdot A^{-1} \cdot C \cdot A^{-1}$$

$$= A^{-1} \cdot (\Sigma_o + m \cdot A^{-1}/2\pi) + m \cdot A^{-1} \cdot J \cdot A^{-1} \qquad \text{E33.a}$$

$$= 2\pi \cdot \begin{pmatrix} (\Sigma_o + m/n^-)n^- & -m/(n^- \cdot n^+) \\ -m/(n^- \cdot n^+) & (\Sigma_o + m/n^+)/n^+ \end{pmatrix} . \qquad \text{E33.b}$$

Defining $F_- = \sum_\beta \cdot G_{-\beta}$ and $F_+ = \sum_\beta \cdot G_\beta$,

and substituting this into E12, we get

$$F_- = G^o_{--} + G^o_{--} \cdot M_{-+} \cdot F_+ + G^o_{--} \cdot M_{--} \cdot F_- \qquad \text{E34.a}$$

and $$F_+ = G^o_{++} + G^o_{++} \cdot M_{++} \cdot F_+ + G^o_{++} \cdot M_{+-} \cdot F_- \quad . \qquad \text{E34.b}$$

These two linear equations can easily be solved to give

$$F_- = \begin{vmatrix} G^o_{--} & -G^o_{--} \cdot M_{-+} \\ G^o_{++} & 1-G^o_{++} \cdot M_{++} \end{vmatrix} / \Delta \qquad \text{E35.a}$$

and $$F_+ = \begin{vmatrix} 1-G^o_{--} \cdot M_{--} & G^o_{--} \\ -G^o_{++} \cdot M_{+-} & G^o_{++} \end{vmatrix} / \Delta \qquad \text{E35.b}$$

where $$\Delta = \begin{vmatrix} 1-G^o_{--} \cdot M_{--} & -G^o_{--} \cdot M_{-+} \\ -G^o_{++} \cdot M_{+-} & 1-G^o_{++} \cdot M_{+-} \end{vmatrix}$$

We find that $$G = F_- + F_+ = \begin{vmatrix} G^o_{--} & -(1-G^o_{--} \cdot (M_{--}-M_{-+})) \\ G^o_{++} & 1-G^o_{++} \cdot (M_{++}-M_{+-}) \end{vmatrix} / \Delta \qquad \text{E36}$$

$$= \frac{G^{o^{-1}}_{++} - (M_{++} - M_{+-}) + G^{o-1}_{--} - (M_{--} - M_{-+})}{(G^{o-1}_{--} - M_{--}).(G^{o-1}_{++} - M_{++}) - M_{+-}.M_{-+}} \quad , \qquad E37$$

where $(M_{--} - M_{-+})/2\pi = (\Sigma_o + m/(n^-.n^+))/n^-$,

$$(M_{++} - M_{-+})/2\pi = (\Sigma_o + m/(n^-.n^+))/n^+ \qquad E38$$

and $(M_{+-}.M_{-+})2\pi = (m/(n^-.n^+))^2$

E37 is therefore equivalent to E32. This method of solving gives us the relation

$$\Gamma^{\ell\ell}_{\ell\ell\sigma} = F_+ \quad \text{and} \quad G^{\sigma}_{\ell\ell} = F_- + F_+ \qquad E39$$

$$F_- = G^{\sigma}_{\ell\ell} - \Gamma^{\ell\ell}_{\ell\ell\sigma} \qquad E40$$

Using E34.b, we have

$$\Gamma^{\ell\ell}_{\ell\ell\sigma} = \frac{G^{o}_{++}.(1 + M_{+-}.G^{\sigma}_{\ell\ell})}{1 - G^{o}_{++}.(M_{++} - M_{+-})} \qquad E41$$

Appendix F

THE SELF-ENERGY $\Sigma_o(\omega)$.

This self-energy function comes directly from the admixing process as has been shown in section 3.5. From expression 3.6.3.a and b we can evaluate the real and imaginary part. To evaluate the imaginary part, $\Delta_o(\omega)$, we use the relation

$$\Delta(\omega) = \pi . \int_{\epsilon_0}^{\epsilon_F} d\epsilon_k . \rho_o(\epsilon_k) . |V_{\ell k}|^2 . \delta(\omega - \epsilon_k) \qquad \text{(F1)}$$

This can be evaluated easily if we can express $|V_{\ell k}|^2$ as function of ϵ_k. From definition (see section 3.4) $V_{\ell k}$ is difficult to evaluate . For simple cubic SIC, we have shown that the wave function $\Psi_k(r)$ is given in 4.2.32, and the matrix element $V_{\ell k}$ is

$$V_{\ell k} = \frac{i}{P} . \sqrt{\frac{2}{M+1}} . \sum_{j} \sum_{\ell j} . \sin(M-j)\Theta . \exp(-ik . \bar{R}_{\ell_j}) . V_\ell(\bar{R}_{\ell_j} + \bar{Z}) \qquad \text{F2}$$

$$= i . \sqrt{\frac{2}{M+1}} . \sum_j . \sin(M-j)\Theta v_{\ell j} , \qquad \text{F3}$$

where $v_{\ell j} = \frac{1}{P} . \sum_{\ell_j} . \exp(-i\bar{k} . \bar{R}_{\ell_j}) . V_\ell(\bar{R}_{\ell_j} + \bar{Z}_j)$, which F4

has the meaning of the coupling between adatom and the j-layer parallel to the surface plane. Since $(M+1)\Theta = n\pi + \delta$

for small surface perturbation (see 4.2.15), we can express 5.4.3 as

$$V_{\ell k} = -i.\sqrt{\frac{2}{M+1}} . \sum_{j} .(-1)^{n}.\sin((j+1)\theta-\delta).v_{\ell j} \quad F5$$

$$= -i.\sqrt{\frac{2}{M+1}} . \sum_{j} .(-1)^{n}.\left[\sin(j+1)\theta.\cos\delta - \cos(j+1)\theta.\sin\delta\right].v_{\ell j}, \quad F6$$

Expressing $\sin(j+1)\theta$ and $\cos(j+1)\theta$ as function of $x\cos\theta$, we can write

j	$\cos(j+1)\theta$	$\sin(j+1)\theta$
0	$\cos\theta$	$1-\cos^2\theta$
1	$2\cos^2\theta-1$	$2\cos\theta\sqrt{1-\cos^2\theta}$
2	$4\cos^3\theta-3\cos\theta$	$(4\cos^2\theta-1)\sqrt{1-\cos^2\theta}$
.	....	....

For large j, $v_{\ell j}$ becomes zero, so that we need to sum only a few term.

There are many configuration that the location of adatoms relates to j layer in the two dimention structure. It can be classified into three main categories as show in Fig.F1.a and b

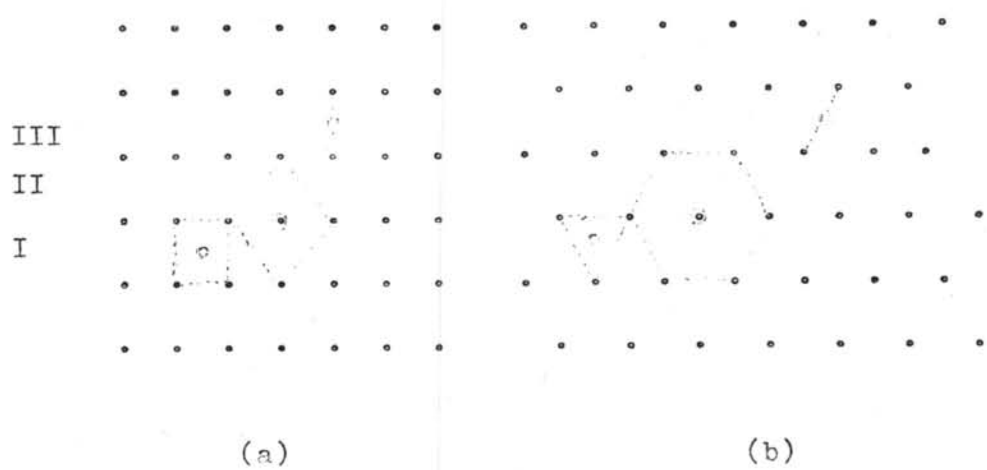


Fig. F1 The relative configuration of adatom ○ to the j layer

a) squarelattice, b) hexagonal lattice.

The configuration would be called adsorption site when j=0 (surface layer). As an example the explicit expansion of $v_{\ell j}$ of square lattice can be written as

$$v^{i}_{\ell j} = 2\bar{v}_{\ell j}(1).\{\cos(k_x.R/2).\cos(k_y.R/2)\} + 2\bar{v}_{\ell j}(2).\{\cos(3k_x.R/2).\cos(k_y.R/2)+\cos(k_x.R/2).\cos(3k_y.R/2)\} + 2\bar{v}_{\ell j}(3).\{.\cos(3k_x.R/2).\cos(3k_y.R/2)\} + 2\bar{v}_{\ell j}(4).\{\cos(5k_x.R/2).\cos(k_y.R/2) + \cos(k_x.R/2).\cos(5k_y.R/2)\} + \ldots\ldots ; \qquad F7.a$$

$$v^{ii}_{\ell j} = \bar{v}'_{\ell j}(0) + 2\bar{v}'_{\ell j}(1).\{\cos(k_x.R) + \cos(k_y.R)\} + 2\bar{v}'_{j}(2).\cos(k_x.R).\cos(k_y.R) + 2\bar{v}'_{\ell j}(3).\{\cos(2k_x.R)+\cos(2k_y.R)\} + 2\bar{v}'_{\ell j}(4).\{\cos(2k_x.R).\cos(k_y.R) + \cos(k_x.R).\cos(2k_y.R)\} + \ldots\ldots\ldots\ldots , \qquad F7.b$$

$$v_{\ell j}^{iii} = 2\bar{v}''_{\ell j}(1).\cos(k_x.R/2) + 2\bar{v}''_{\ell j}(2).\cos(k_x.R/2).\cos(k_y.R)$$

$$+ 2\bar{v}''_{\ell j}(3).\cos(3k_x.R/2) + 2\bar{v}'j(4).\cos(3k_x.R/2).\cos(k_y.R) + .$$

$$..............; \qquad F7.c$$

where $v_{\ell j}^{i,ii,iii}$ are corresponded to the type I,II,III respectively. This can be worked out for the two dimention lattice. If the phase shift δ is known F6 can be evaluated. We shall find that this phase shift is small and can be set equal to zero. So that

$$|V_{\ell k}|^2 = \frac{2}{M+1}. \sum_{jj'} .\sin(j+1)\theta.\sin(j'+1)\theta.V^*_{\ell j}.V_{\ell j'} \qquad F8$$

$$= \frac{2}{M+1}.(1-\cos^2\theta).f(k_x,k_y,\theta), \qquad F9$$

$$\text{where } f(k_x,k_y,\theta) = (\sum_j .g_j(\theta).v_{\ell j}(k_x,k_y))^2 , \qquad F10$$

$$\text{Defining } \sin(j+1)\theta = (1-\cos^2\theta)^{\frac{1}{2}}.g_j(\theta) , \qquad F11$$

we find that $g_j(\theta)$ is equal to 1, $2\cos\theta$ and $4\cos^2\theta-1$ etc., when j equal to 0,1 and 2 etc.. Unfortunately, we cannot give any detail analysis of the f-function for the three-dimensional crystal. However, $\Delta_o(\omega)$ can be worked numerically, which is shown schematically in appendix G.

The most frequently used crystal model to study chemisorption is one-dimensional SIC. without any surface perturbation (the ideal). For this model, let us consider the type II. $\bar{v}'_{\ell j}(i)$ is zero for all i greater than zero, so that

$$f(\theta) = (\sum_j . g_j(\theta) . \bar{v}'_{\ell j}(0))^2 \quad . \qquad F12$$

To see the corresponding rsult of one-dimensional model to Newns'semi-elliptic $\Delta_o(\omega)$, we assume the same assumtion that $\bar{v}'_{\ell j}(0) = \bar{v}'_{\ell o}(0) . \delta_{oj}$.

Then $$f(\theta) = |\bar{v}'_{\ell o}(0)|^2 \qquad F13$$

where $$|V_{\ell k}|^2 = \frac{2}{M+1} . (1-\cos^2\theta) . |\bar{v}'_{\ell o}(0)|^2 \qquad F14$$

Since we have $$\varepsilon_k = \alpha - 2|\beta| . \cos\theta$$

and $$\rho_o(\varepsilon_k) = \frac{M+1}{\pi} . \frac{d\theta}{d\varepsilon_k} = \frac{M+1}{2\pi|\beta| . \sqrt{1-\cos^2\theta}} , \qquad F15$$

Defining $$x = \frac{\varepsilon_k - \alpha}{2|\beta|} , \qquad F16$$

and applying this to F14 and F15 as well as putting this into F1, we h

$$\Delta_o(x) = \Delta_o(\omega)/(2|\beta|)^2$$

$$= \pi . \int_{-1}^{+1} d\bar{x} . \frac{M+1}{\pi . \sqrt{1-\bar{x}^2}} . \frac{2}{M+1} . (1-\bar{x}^2) . \lambda^2 . \delta(x-\bar{x})$$

$$= 2\lambda^2 . \sqrt{1-x^2} , \qquad F17$$

where $$= |v_{\ell o}(0)| / 2|\beta| \quad . \qquad F18$$

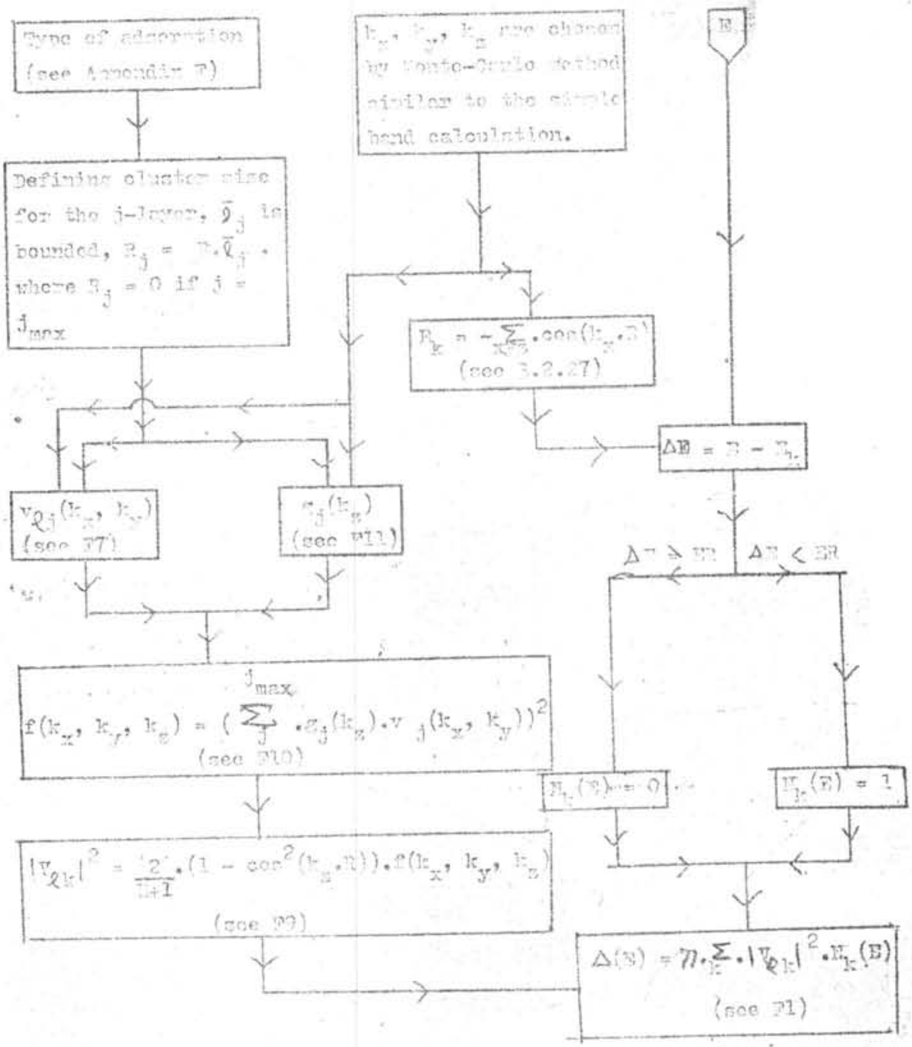
Then
$$\Lambda_o(x) = \Lambda_o(\omega)/(2|\beta|)^2$$
$$= \frac{2\lambda^2}{\pi} . P \int_{-1}^{+1} d\bar{x} . \frac{\sqrt{1-\bar{x}^2}}{x-\bar{x}}$$
$$= 2\lambda^2 . (x - sig(x) . \sqrt{1-x^2} . \theta(|x|-1) \quad , \quad F19$$

where θ (u) is the step function which is zero when u < 0 and is equal to unity when u > 0 ,

This show that our three-dimentional model has one-dementional limit which is equivalent to the result to those Nenws' one-dimentional model.

APPENDIX G

THE $\Delta_0(E)$ SIMPLE NUMERICAL CALCULATION SCHEME.



VITA

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