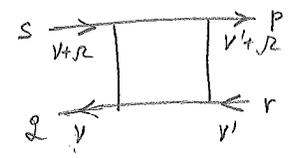


TWO - PARTICLE VERTEX NOTES

For other details see Hyonon's thesis.

Local vertex sampled in ctymc

$$X_{sp;pr} \equiv \langle \psi_p^+(i_1) \psi_f^+(i_2) \psi_r(i_3) \psi_s(i_4) \rangle$$



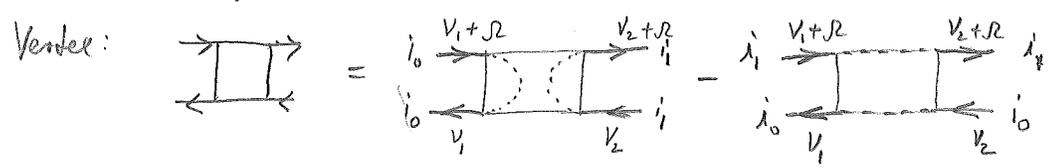
In ctymc we evaluate vertex in the following way:

$$X_H[i_0, i_1; i_2, i_1, i_2] = M[i_0](i_1, i_1 + i_2) M[i_1](i_2 + i_2, i_2)$$

$$X_F[i_0, i_1; i_2, i_1, i_2] = M[i_0](i_1, i_2) M[i_1](i_2 + i_2, i_1 + i_2)$$

where $M[i_0](i_1, i_1) = G_{i_0}(i_1)$ is the one particle Green's function.

Diagrammatically this is:



The vertex can be derived by the formula:

$$\begin{aligned} X_{sp;pr} &= \frac{1}{Z} \frac{\partial^2 Z}{\partial \Delta_{ps} \partial \Delta_{gr}} = \frac{1}{Z} \frac{\partial^2}{\partial \Delta_{ps} \partial \Delta_{gr}} \int \mathcal{D}[\psi^+] e^{-S_{\text{ctymc}} - \int \psi_\alpha^+ \Delta_{\alpha\beta} \psi_\beta} \\ &= \frac{1}{Z} \int \mathcal{D}[\psi^+] e^{-S_{\text{ctymc}}} \psi_p^+ \psi_s \psi_f^+ \psi_r \\ &= \frac{1}{Z} \frac{\partial^2}{\partial \Delta_{ps} \partial \Delta_{gr}} \int \mathcal{D}[\psi^+] e^{-S_{\text{ctymc}}} (\psi_{i_1}^+ \psi_{i_2} \psi_{i_3}^+ \psi_{i_4}) \text{Det}(\Delta) \end{aligned}$$

$$X_{sp;pr} = \frac{1}{Z} \text{Tr}(\psi_{i_1}^+ \psi_{i_2} \psi_{i_3}^+ \psi_{i_4}) \frac{\partial^2}{\partial \Delta_{ps} \partial \Delta_{gr}} \text{Det}(\Delta)$$

In practice, we print out $X - X^0$, where X^0 is bubble. In particular,

$$X^0 \equiv B_H + B_F$$

$$B_H[i_0, i_1, i_2, i_1, i_2] = \delta(R=0) M[i_0](i_1, i_1) M[i_1](i_2, i_2) \equiv \delta(R=0) G_{i_0}(i_1) G_{i_1}(i_2)$$

$$B_F[i_0, i_1, i_2, i_1, i_2] = \delta(v_1=v_2) M[i_0](i_1) M[i_1](i_1 + i_2) \equiv \delta(v_1=v_2) G_{i_0}(i_1) G_{i_1}(i_1 + i_2)$$

Diagrammatically we have:



Magnetic and charge χ

$\chi = \chi_0 + \chi_0 \Gamma \chi$: Dyson equation $\rightarrow \Gamma$ is irreducible vertex
 χ_0 is the bubble

$$\chi_{SS;S'S'} = \chi_{SS}^0 \chi_{SS'} + \chi_{SS}^0 \Gamma_{SS;S''S''} \chi_{S''S'';S'S'}$$

In paramagnetic state we have $\chi_{\uparrow\uparrow;\uparrow\uparrow} = \chi_{\downarrow\downarrow;\downarrow\downarrow}$ and $\chi_{\uparrow\uparrow;\downarrow\downarrow} = \chi_{\downarrow\downarrow;\uparrow\uparrow}$ hence

$$\chi_{\uparrow\uparrow;\uparrow\uparrow} = \chi_{\uparrow\uparrow}^0 + \chi_{\uparrow\uparrow}^0 (\Gamma_{\uparrow\uparrow;\uparrow\uparrow} \chi_{\uparrow\uparrow;\uparrow\uparrow} + \Gamma_{\uparrow\uparrow;\downarrow\downarrow} \chi_{\downarrow\downarrow;\uparrow\uparrow})$$

$$\chi_{\uparrow\uparrow;\downarrow\downarrow} = \phi + \chi_{\uparrow\uparrow}^0 (\Gamma_{\uparrow\uparrow;\uparrow\uparrow} \chi_{\uparrow\uparrow;\downarrow\downarrow} + \Gamma_{\uparrow\uparrow;\downarrow\downarrow} \chi_{\downarrow\downarrow;\downarrow\downarrow})$$

we have:

$$\chi_{\uparrow\uparrow;\uparrow\uparrow} \pm \chi_{\uparrow\uparrow;\downarrow\downarrow} = \chi_{\uparrow\uparrow}^0 + \chi_{\uparrow\uparrow}^0 \left\{ \Gamma_{\uparrow\uparrow;\uparrow\uparrow} (\chi_{\uparrow\uparrow;\uparrow\uparrow} \pm \chi_{\uparrow\uparrow;\downarrow\downarrow}) + \Gamma_{\uparrow\uparrow;\downarrow\downarrow} (\chi_{\downarrow\downarrow;\uparrow\uparrow} \pm \chi_{\downarrow\downarrow;\downarrow\downarrow}) \right\}$$

$$\chi^d = \chi_{\uparrow\uparrow\uparrow\uparrow} + \chi_{\uparrow\uparrow\downarrow\downarrow} \quad \text{and} \quad \Gamma^m = \chi_{\uparrow\uparrow\uparrow\uparrow} - \chi_{\uparrow\uparrow\downarrow\downarrow}$$

$$\Gamma^d = \Gamma_{\uparrow\uparrow\uparrow\uparrow} + \Gamma_{\uparrow\uparrow\downarrow\downarrow} \quad \text{and} \quad \Gamma^m = \Gamma_{\uparrow\uparrow\uparrow\uparrow} - \Gamma_{\uparrow\uparrow\downarrow\downarrow}$$

finally:

$$\chi^m = \chi^0 + \chi^0 \Gamma^m \chi^m$$

$$\chi^d = \chi^0 + \chi^0 \Gamma^d \chi^d$$

In paramagnetic state we compute $\langle M^z(\tau) M^z(0) \rangle$. If spin-orbit is small, we have $\langle S^z(\tau) S^z(0) \rangle$

$$\chi^{zz} = \sum_{\alpha\beta} (\chi_{\alpha\uparrow\alpha\uparrow;\beta\uparrow\beta\uparrow} + \chi_{\alpha\downarrow\alpha\downarrow;\beta\downarrow\beta\downarrow} - \chi_{\alpha\uparrow\alpha\uparrow;\beta\downarrow\beta\downarrow} - \chi_{\alpha\downarrow\alpha\downarrow;\beta\uparrow\beta\uparrow}) (S^z)^2$$



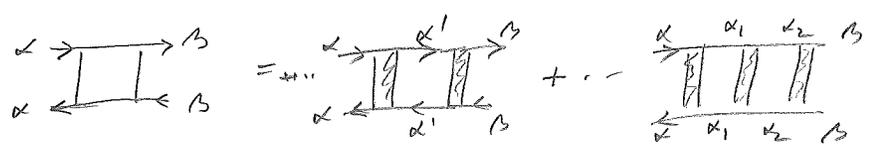
$$= \sum_{\alpha\beta} 2 \chi_{\alpha\alpha\beta\beta}^m \cdot \frac{1}{4}$$

From regime we have

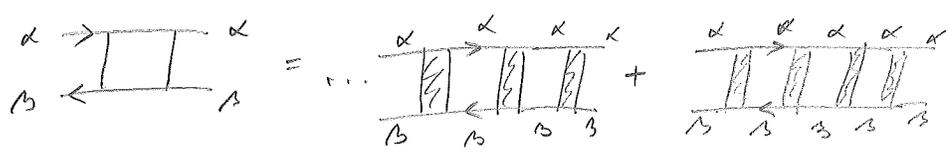
$\chi_{\alpha\alpha\beta\beta}^{impurity}$ and $\chi_{\alpha\beta\alpha\beta}^{impurity}$



If we consider only the z-component of Hund's coupling, we have α as a "good local" quantum number, hence we have



and also



We thus have

$$\chi_{\alpha_1\alpha_2;\beta_1\beta_2} = \chi_{\alpha\alpha;\beta\beta}^{(1)} \int_{\alpha_1=\alpha} \int_{\beta_1=\beta_2} + \chi_{\alpha\beta;\alpha\beta}^{(2)} \int_{\alpha_1=\beta_1=\alpha} \int_{\alpha_2=\beta_2=\beta}$$

The impurity susceptibility $\chi^{(1)}$ and $\chi^{(2)}$ satisfy:

$$\chi_{\alpha\alpha;\beta\beta}^{(1)} = \chi_{\alpha\alpha}^0 \int_{\alpha\beta} - \chi_{\alpha\alpha}^0 \Gamma_{\alpha\alpha\alpha'\alpha'} \chi_{\alpha'\alpha';\beta\beta}^{(1)}$$

hence we invert matrix in frequency $\nu\nu'$ and orbitals $\alpha\beta$ to obtain

$$(\Gamma^{(1)})_{\alpha\alpha\nu;\beta\beta\nu'} = (\chi^{-1} - \chi_0^{-1})^{-1}_{\alpha\alpha\nu;\beta\beta\nu'}$$

For $\chi_{\alpha\beta;\alpha\beta}^{(2)}$ when $\alpha \neq \beta$ we simply have

$$\chi_{\alpha\beta;\alpha\beta}^{(2)} = \chi_{\alpha\beta;\alpha\beta}^0 - \chi_{\alpha\beta;\alpha\beta}^0 \Gamma_{\alpha\beta\alpha\beta} \chi_{\alpha\beta;\alpha\beta}^{(2)}$$

hence we have matrix multiplication only in frequency ν and ν' but not in orbital index. We thus have:

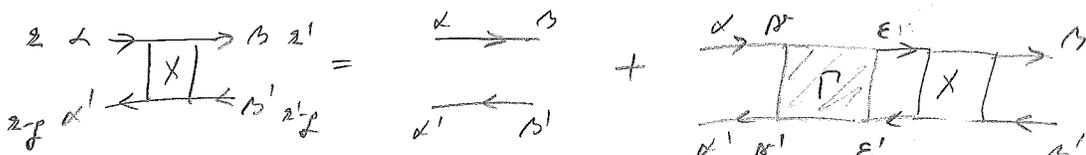
$$\Gamma_{\alpha\beta;\alpha\beta}^{(2)} = (\chi_{\alpha\beta;\alpha\beta}^{-1} - \chi_{\alpha\beta;\alpha\beta}^{0-1})^{-1}$$

with matrices in frequency only

↑ here $\alpha \neq \beta$ to avoid double-counting

To compute g -dependent susceptibility, we need to work with all 4 orbital index λ .

(4)



$$\chi_{\alpha\alpha', \beta\beta'}^{z, z'} = \chi_{\alpha\alpha', \beta\beta'}^{0, z} - \sum_{\epsilon, \epsilon'} \chi_{\alpha\alpha', \beta\beta'}^{0, z} \Gamma_{\alpha\alpha', \beta\beta'}^{\epsilon, \epsilon'} \chi_{\epsilon\epsilon', \beta\beta'}^{z, z'}$$

Since Π is momentum independent, we can sum over internal momenta and define

$$\chi_{\alpha\alpha', \beta\beta'}^{0, z} = \sum_{\alpha} \chi_{\alpha\alpha', \beta\beta'}^{0, z} = \sum_{\alpha} G_{\beta\alpha}^z(i\nu) G_{\alpha\beta'}^{z-p}(i\nu - iR)$$

hence we have only momentum g as parameter. We keep full frequency dependence and orbital dependence.

We define combined index $(\alpha\alpha', \nu)$ and write

$$\chi_{(\alpha\alpha', \nu), (\beta\beta', \nu)}^{z, z'} = [\chi_{g, R}^{0, z} - \Gamma_{z, z'}]^{-1} \quad \text{here } g \text{ and } R \text{ are parameters}$$

On real axis we need $\chi_g^0(R)$ which is

$$\chi_{\alpha\alpha', \beta\beta'}^0(iR) = -\frac{1}{\beta} \sum_{\alpha} G_{\beta\alpha}^z(i\nu) G_{\alpha\beta'}^{z-p}(i\nu - iR) = \int \frac{d^2z}{2\pi^2} f(z) G_{\beta\alpha}^z(z) G_{\alpha\beta'}^{z-p}(z - iR)$$

$$\chi_g^0(iR) = \int \frac{d^2x}{2\pi^2} [f(x) [G_{\beta\alpha}^z(x+i\delta) - G_{\beta\alpha}^z(x-i\delta)] G_{\alpha\beta'}^{z-p}(x-iR) + f(x+iR) G_{\beta\alpha}^z(x+iR) [G_{\alpha\beta'}^{z-p}(x+i\delta) - G_{\alpha\beta'}^{z-p}(x-i\delta)]]$$

$$\frac{1}{2i} [\chi_g^0(R+i\delta) - \chi_g^0(R-i\delta)] \equiv \chi_g^{0||}(R) = \int \frac{d^2x}{\pi} f(x) \left[\frac{1}{2i} (G_{\beta\alpha}^z(x) - G_{\beta\alpha}^+(x)) \frac{1}{2i} (G_{\alpha\beta'}^{z-p}(x-R) - G_{\alpha\beta'}^{z-p}(x-R)) + \frac{1}{2i} (G_{\beta\alpha}^z(x+R) - G_{\beta\alpha}^+(x+R)) \frac{1}{2i} (G_{\alpha\beta'}^{z-p}(x) - G_{\alpha\beta'}^+(x)) \right]$$

Define: $\rho_{\beta\alpha}^z(x) = \frac{1}{2i} (G_{\beta\alpha}^z(x) - G_{\beta\alpha}^+(x))$

$$\chi_g^{0||}(\beta) = \int \frac{d^2x}{\pi} [f(x-R) - f(x)] \rho_{\beta\alpha}^z(x) \rho_{\alpha\beta'}^{z-p}(x-R)$$

The complex form of the Kronen-Kronig relation can be used to obtain full χ^0

$$\frac{1}{2} [\chi(\omega + i\delta) - \chi(\omega - i\delta)] = -\frac{1}{\pi} \mathcal{P} \int_{-\infty}^{\infty} \frac{\frac{1}{2i} [\chi(x + i\delta) - \chi(x - i\delta)]}{\omega - x} dx$$

Some notes on cyclic implementation:

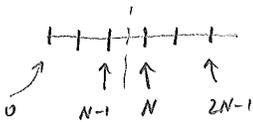
fermionic frequency

$m = 0$	$V = -\frac{(2N-1)\pi}{\Lambda}$
\vdots	\vdots
$m = N_w - 1$	$V = -\frac{\pi}{\Lambda}$
$m = N_w$	$V = \frac{\pi}{\Lambda}$
\vdots	\vdots
$m = 2N_w - 1$	$V = \frac{(2N-1)\pi}{\Lambda}$

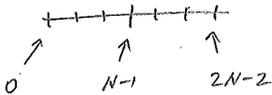
bosonic frequency

$iR = 0$	$dR = N_R - 1$	$R = -2(N-1)\pi/\Lambda$
\vdots	\vdots	\vdots
$iR = N_R - 1$	$dR = 0$	$R = 0$
$iR = N_R$	$dR = 1$	$R = 2\pi/\Lambda$
\vdots	\vdots	\vdots
$iR = 2N_R - 2$	$dR = -N_R + 1$	$R = 2(N-1)\pi/\Lambda$

index



$$V = \frac{\pi}{\Lambda} (-(2N_w - 1) + 2m)$$



$$R = dR \frac{2\pi}{\Lambda}$$

$m + dR$ represents

$$\frac{\pi}{\Lambda} (-(2N_w - 1) + 2m) + dR \frac{2\pi}{\Lambda} = \frac{\pi}{\Lambda} (-(2N_w - 1) + 2(m + dR))$$

$$iR \in [0, \dots, 2N_R - 1] \rightarrow R = -2(N_R - 1)\frac{\pi}{\Lambda}, \dots, 2(N_R - 1)\frac{\pi}{\Lambda}$$

$$im_1 \in \max(0, -dR), \min(2N_w, 2N_w - dR)$$

$$im_2 \in \max(0, -dR), \min(2N_w, 2N_w - dR)$$

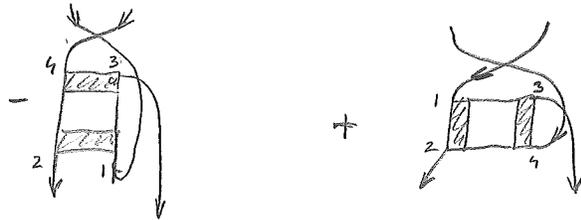
Superconductivity

We will construct particle-particle irreducible vertex from particle hole reducible diagrams. More specifically

$$\begin{array}{c}
 \text{irreducible} \\
 \text{vertex in p-p} \\
 \text{channel}
 \end{array}
 = - \text{diagram 1} + \text{diagram 2}$$

$(\Gamma \chi \Gamma)^{p-h-1}$ $(\Gamma \chi \Gamma)^{p-h-2}$

These two diagrams can be replotted in the following equivalent form:



We are interested in spin-singlet pairing, hence we compute:

$$\Gamma_{\text{singlet}}^{pp} = \frac{1}{2} (\Gamma_{\uparrow\downarrow\uparrow\downarrow} - \Gamma_{\uparrow\downarrow\downarrow\uparrow})$$

We thus have:

$$\Gamma_{pp}^{(1)} = -\frac{1}{2} \left[\text{diagram 1} - \text{diagram 2} \right] = -\frac{1}{2} \left[(\Gamma \chi \Gamma)^{ph}(\uparrow\downarrow\downarrow\uparrow) - (\Gamma \chi \Gamma)^{ph}(\downarrow\uparrow\uparrow\downarrow) \right]$$

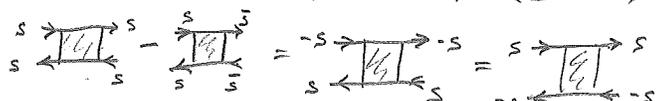
$$\Gamma_{pp}^{(2)} = \frac{1}{2} \left[\text{diagram 3} - \text{diagram 4} \right] = \frac{1}{2} \left[(\Gamma \chi \Gamma)^{ph}(\downarrow\uparrow\downarrow\uparrow) - (\Gamma \chi \Gamma)^{ph}(\uparrow\downarrow\downarrow\uparrow) \right]$$

From definition of χ^m and χ^d it follows: $(\Gamma \chi \Gamma)(\uparrow\downarrow\downarrow\uparrow) = \frac{1}{2} [(\Gamma \chi \Gamma)^d - (\Gamma \chi \Gamma)^m]$

In paramagnetic state we have special symmetry

hence

$$\langle S^z(\tau) S^z \rangle = \langle S^+(\tau) S^- \rangle = \langle S^-(\tau) S^+ \rangle$$

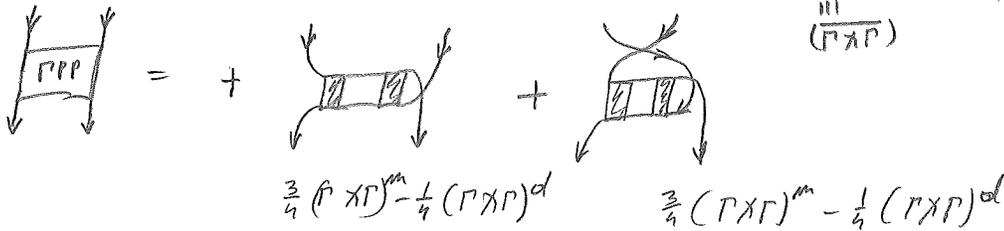


$$\text{or } \chi_{\downarrow\uparrow\downarrow\uparrow}^{ph} = \chi_{\uparrow\uparrow\uparrow\uparrow}^{ph} - \chi_{\uparrow\downarrow\uparrow\downarrow}^{ph} \equiv \chi^m$$

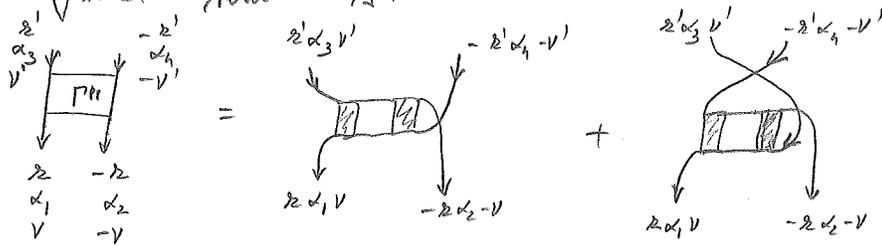
We thus have: $\Gamma^{PP(1)} = -\frac{1}{2} \left[\frac{1}{2} (\Gamma \chi \Gamma)^{ol} - \frac{1}{2} (\Gamma \chi \Gamma)^m - (\Gamma \chi \Gamma)^m \right] = -\frac{1}{4} (\Gamma \chi \Gamma)^{ol} + \frac{3}{4} (\Gamma \chi \Gamma)^m$ (7)

$\Gamma^{PP(2)} = \frac{1}{2} \left[(\Gamma \chi \Gamma)^m - \frac{1}{2} (\Gamma \chi \Gamma)^{ol} + \frac{1}{2} (\Gamma \chi \Gamma)^m \right] = \frac{3}{4} (\Gamma \chi \Gamma)^m - \frac{1}{4} (\Gamma \chi \Gamma)^{ol}$

We just proved that for the simplest pairing, we can drop the spin indices and use the block $\frac{3}{4} (\Gamma \chi \Gamma)^m - \frac{1}{4} (\Gamma \chi \Gamma)^{ol}$ as the building block:



The final result is:



$\Gamma^{PP}(\alpha_1, \alpha_2, 2v; \alpha_3, \alpha_4, 2v') = (\overline{\Gamma \chi \Gamma})_{2-2}^{ph}(\alpha_3, \alpha_4, v'; \alpha_2, \alpha_1, -v) + (\overline{\Gamma \chi \Gamma})_{-2-2}^{ph}(\alpha_4, \alpha_1, -v'; \alpha_2, \alpha_3, -v)$

where $(\overline{\Gamma \chi \Gamma})^{ph} = \frac{3}{4} (\Gamma \chi \Gamma)^m - \frac{1}{4} (\Gamma \chi \Gamma)^{ol}$

The Eliashberg equation reads:

$$-\frac{1}{\beta} \sum_{\substack{\alpha_1, \alpha_2, \alpha_3, \alpha_4 \\ v, v'}} \Gamma^{PP}(\alpha_1, \alpha_2, 2iv; \alpha_3, \alpha_4, 2iv') \chi_{2v'}^{0P-P}(\alpha_3, \alpha_4, \alpha_5, \alpha_6) \phi_{\alpha_5, \alpha_6}^{2v'} = \lambda \phi_{\alpha_1, \alpha_2}^{2v}$$

BCS approximation amounts to letting all frequency in Γ^{PP} to zero on real axis.

$\Gamma^{PP}(\alpha_1, \alpha_2, 2v; \alpha_3, \alpha_4, 2v') \approx \Gamma^{PP}(\alpha_1, \alpha_2, 2^+ 0^+; \alpha_3, \alpha_4, 2^+ 0^+)$ hence we have

$$-\sum_{\alpha_1, \alpha_2, \alpha_3, \alpha_4} \Gamma^{PP}(\alpha_1, \alpha_2, 2^+ 0^+; \alpha_3, \alpha_4, 2^+ 0^+) \left(\frac{1}{\beta} \sum_{iv'} \chi_{iv'}^{0P-P}(\alpha_3, \alpha_4, \alpha_5, \alpha_6, 2^+) \right) \phi_{\alpha_5, \alpha_6}^{2^+} = \lambda \phi_{\alpha_1, \alpha_2}^{2^+}$$

where

$\frac{1}{\beta} \sum_{iv} \chi_{iv}^{0P-P}(\alpha_3, \alpha_4, 2; \alpha_5, \alpha_6, 2) = \frac{1}{\beta} \sum_{iv} G_{\alpha_3, \alpha_5}^2(iv) G_{\alpha_4, \alpha_6}^{-2}(-iv)$; $\sqrt{\frac{v_5 v_6}{v_2 v_4}}$

We are here diagonalizing

$$-\sum_{\alpha_3 \alpha_4} \Gamma^{PP}(\alpha_1 \alpha_2 z 0^+; \alpha_3 \alpha_4 z' 0^+) \chi^{PP-P}(\alpha_3 \alpha_4 z'; \alpha_1 \alpha_2 z') \equiv \mathcal{E}(\alpha_1 \alpha_2 z; \alpha_1 \alpha_2 z')$$

Here

$$\Gamma^{PP}(\alpha_1 \alpha_2 z 0^+; \alpha_3 \alpha_4 z' 0^+) = (\overline{\Gamma \chi \Gamma})_{\substack{z'-z \\ z=0}}^{ph}(\alpha_3 \alpha_4 0^+; \alpha_1 \alpha_2 0^-) + (\overline{\Gamma \chi \Gamma})_{\substack{-z'-z \\ z=0}}^{ph}(\alpha_4 \alpha_1 0^-; \alpha_2 \alpha_3 0^-) (XY)$$

What is symmetric?

Time reversal symmetry gives: $G_{\alpha\beta}^z(i\omega) = G_{\beta\alpha}^{-z}(i\omega) = G_{\alpha\beta}^{-z*}(-i\omega)$
 because $G^z(-i\omega) = G_{(i\omega)}^{z+}$

We can show for bubble:

$$1) \chi_{\beta}^0(\alpha_1 \alpha_2; \alpha_3 \alpha_4) = \chi_{-\beta}^0(\alpha_3 \alpha_4; \alpha_1 \alpha_2)$$

$$2) \chi_{\beta}^0(\alpha_1 \alpha_2; \alpha_3 \alpha_4) = \chi_{\beta}^0(\alpha_2 \alpha_1; \alpha_4 \alpha_3)$$

(iν iν', iρ) (iν-iρ, iν'-iρ, iρ)

Hermitian conjugate of $E_{\beta}(XY)$ is

$$\Gamma^{PP}(\alpha_3 \alpha_4 z' 0^+; \alpha_1 \alpha_2 z 0^+)^* = (\overline{\Gamma \chi \Gamma})_{-(z'-z)}^{ph*}(\alpha_1 \alpha_3 0^+; \alpha_4 \alpha_2 0^-) + (\overline{\Gamma \chi \Gamma})_{-z'-z}^{ph*}(\alpha_2 \alpha_3 0^-; \alpha_4 \alpha_1 0^-)$$

If solution $\phi^z = \phi^{-z}$, we can use $\Gamma^{PP}(\alpha_1 \alpha_2 -z 0^+; \alpha_3 \alpha_4 z' 0^+)$ instead of $\Gamma^{PP}(\alpha_1 \alpha_2 z 0^+; \alpha_3 \alpha_4 z' 0^+)$

The vertex is then symmetric. But only for BCs and symmetric in z solution.