If one considers the much stronger anisotropic interactions[7-10] between rare-earth and iron ions, far less than 1% preferential pairing is probably required.

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Pair-Preference and Site-Preference Models for Rare-Earth Iron Garnets Exhibiting Noncubic Magnetic Anisotropies

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The pair anisotropy model is extended to include the next-nearest-neighbor tetrahedral-iron ions. An anisotropy model based on growth-induced preferential site occupation is derived using the pair model. With the site model the nearest-neighbor tetrahedral- and nearest-neighbor octahedral-iron ions lead solely to a uniaxial anisotropy under both growth facets. Inclusion of the next-nearest-neighbor tetrahedral-iron ions results in the experimentally observed orthorhombic anisotropies.

Recent experiments on flux-grown magnetic garnets containing two or more rare earths have shown that some of these garnets exhibit noncubic magnetic anisotropies of the order of 10^4 erg/cm^3 at room temperature.[1] We have earlier proposed a pair-anisotropy model[2] based on the possible existence of a growth-induced preferential pair ordering between the rare-earth ions and their nearest-neighbor tetrahedral-iron (NNT) and nearest-neighbor octahedral-iron (NNO) ions. This model has been shown to predict the observed symmetries of the noncubic anisotropies,[2] and to give good quantitative agreement with room-temperature torque measurements recently performed on a series of these garnets.[3]

In this Letter we extend the pair model to include the next-nearest-neighbor tetrahedral-iron (NNNT) ions as well. Although the NNNT ions are farther from the rare-earth site than the NNT ions, the anisotropic superexchange between the rare earths and the NNNT ions is comparable to if not larger than that with the NNO ions.[4,5] In addition we derive, with help of the pair-preference model, a site-preference model in which we assume a growth-induced preferential site occupation of the rare-earth ions in the dodecahedral sublattice. We show that, unlike the pair-preference model, the site-preference model predicts only a uniaxial anisotropy when the NNNT ions are not considered. However, when these ions are considered, the site-preference model predicts the same orthorhombic symmetries for the induced anisotropies as does the pair-preference model.

We consider a garnet crystal having two rare-earth ions, A and B, in the dodecahedral sublattice and the iron ions C in the tetrahedral and octahedral sublattices. Each rare-earth ion is bonded to (i) two NNT ions by $\langle 100 \rangle$ bonds, (ii) four NNO ions by $\langle 210 \rangle$ bonds, and (iii) four NNT ions

by $\langle 211 \rangle$ bonds, where the above sequence of neighbors is in order of increasing distance. Using the procedure outlined in Refs. 2 and 3, we find that the pair-preference model predicts the growth-induced pair anisotropy under the (110) facet (when written in the $\{110\}$ coordinate system where $x \equiv [001]$, $y \equiv [1\bar{1}0]$, and $z \equiv [110]$) to be

$$E_{(110)}{}^p = 2(N_{AC}l_0)^{\mathrm{I}}(\epsilon_0{}^{\mathrm{I}} - \epsilon_1{}^{\mathrm{I}})(\alpha_x{}^2 - \tfrac{1}{3}) + \tfrac{2}{5}(N_{AC}l_0)^{\mathrm{II}}[\epsilon_1{}^{\mathrm{II}}(16\alpha_x{}^2 + 11\alpha_y{}^2 + 3\alpha_z{}^2) + \epsilon_2{}^{\mathrm{II}}(4\alpha_x{}^2 + 8\alpha_y{}^2 + 8\alpha_z{}^2) + \epsilon_3{}^{\mathrm{II}}(\alpha_y{}^2 + 9\alpha_z{}^2)]$$

$$+ \tfrac{1}{3}(N_{AC}l_0)^{\mathrm{III}}[\epsilon_0{}^{\mathrm{III}}(8\alpha_x{}^2 + 4\alpha_y{}^2) + \epsilon_1{}^{\mathrm{III}}(4\alpha_x{}^2 + 18\alpha_y{}^2 + 2\alpha_z{}^2)$$

$$+ \epsilon_2{}^{\mathrm{III}}(8\alpha_x{}^2 + 4\alpha_z{}^2) + \epsilon_3{}^{\mathrm{III}}(4\alpha_x{}^2 + 2\alpha_y{}^2 + 18\alpha_z{}^2)] + C_1. \tag{1}$$

In Eq. (1) the magnetization has direction cosines $(\alpha_x, \alpha_y, \alpha_z)$ and the superscripts I, II, and III designate the parameters for $\langle 100 \rangle$, $\langle 210 \rangle$, and $\langle 211 \rangle$ pair ordering, respectively. The total number of AC bonds per unit volume is given by N_{AC}. The term $l_0 = l_{AC} - l_{BC}$ is the net pair-interaction coefficient. The preference parameters $\epsilon^{\mathrm{I,II,III}}$ represent the relative preference for each of the different AC bonds of types I, II, and III. Equation (1) defines an orthorhombic anisotropy whose principal axes are the principal axes of the $\{110\}$ coordinate system. This is the observed anisotropy.[2,3]

Similarly under the (112) growth facet the pair anisotropy (when written in the $\{112\}$ coordinate system where $x \equiv [11\bar{1}]$, $y \equiv [\bar{1}10]$, and $z \equiv [112]$) is

$$E_{(112)}{}^p = \tfrac{2}{3}(N_{AC}l_0)^{\mathrm{I}}(\epsilon_2{}^{\mathrm{I}} - \epsilon_1{}^{\mathrm{I}})[\alpha_x{}^2 + 2\alpha_z{}^2 - (2\sqrt{2})\alpha_x\alpha_z - 1] + \tfrac{2}{5}(N_{AC}l_0)^{\mathrm{II}}[\epsilon_0{}^{\mathrm{II}}(6\alpha_x{}^2 + 4\alpha_y{}^2)$$

$$+ \epsilon_1{}^{\mathrm{II}}(\tfrac{2}{3}\alpha_x{}^2 + 9\alpha_y{}^2 + \tfrac{1}{3}\alpha_z{}^2 + \tfrac{8}{3}\sqrt{2}\alpha_x\alpha_z) + \epsilon_3{}^{\mathrm{II}}(12\alpha_x{}^2 + 2\alpha_y{}^2 + 6\alpha_z{}^2) + \epsilon_4{}^{\mathrm{II}}(\tfrac{2}{3}\alpha_x{}^2 + 4\alpha_y{}^2 + \tfrac{16}{3}\alpha_z{}^2 + \tfrac{8}{3}\sqrt{2}\alpha_x\alpha_z)$$

$$+ \epsilon_5{}^{\mathrm{II}}(\tfrac{2}{3}\alpha_x{}^2 + \alpha_y{}^2 + \tfrac{25}{3}\alpha_z{}^2 - \tfrac{10}{3}\sqrt{2}\alpha_x\alpha_z)] + \tfrac{1}{3}(N_{AC}l_0)^{\mathrm{III}}[\epsilon_1{}^{\mathrm{III}}(\tfrac{40}{3}\alpha_x{}^2 + 10\alpha_y{}^2 + \tfrac{2}{3}\alpha_z{}^2 + \tfrac{4}{3}\sqrt{2}\alpha_x\alpha_z)$$

$$+ \epsilon_2{}^{\mathrm{III}}(\tfrac{16}{3}\alpha_x{}^2 + \tfrac{2}{3}\alpha_z{}^2 - \tfrac{8}{3}\sqrt{2}\alpha_x\alpha_z) + \epsilon_3{}^{\mathrm{III}}(9\alpha_y{}^2 + 3\alpha_z{}^2) + \epsilon_4{}^{\mathrm{III}}(\tfrac{8}{3}\alpha_x{}^2 + 4\alpha_y{}^2 + \tfrac{16}{3}\alpha_z{}^2 - \tfrac{16}{3}\sqrt{2}\alpha_x\alpha_z)$$

$$+ \epsilon_5{}^{\mathrm{III}}(\tfrac{8}{3}\alpha_x{}^2 + \alpha_y{}^2 + \tfrac{25}{3}\alpha_z{}^2 + \tfrac{20}{3}\sqrt{2}\alpha_x\alpha_z) + \epsilon_6{}^{\mathrm{III}}(\tfrac{18}{3}\alpha_z{}^2)] + C_2. \tag{2}$$

Equation (2) defines a noncubic anisotropy under the $\{112\}$ facet with such symmetry that the easy axis will be either along the $[\bar{1}10]$ axis in the (112) plane, or alternatively somewhere in the $(\bar{1}10)$ plane. This again is the observed symmetry.[2,3]

We note that the addition of the $l_0{}^{\mathrm{III}}$ terms, that is, those involving the NNNT ions, does not alter the symmetry of the anisotropy from that derived solely from the $l_0{}^{\mathrm{I}}$ (NNT) plus $l_0{}^{\mathrm{II}}$ (NNO) terms.[2,3] In addition, the inclusion of the $l_0{}^{\mathrm{III}}$ terms produces no appreciable change in the quantitative analysis of Refs. 1 and 2. This last result is not surprising in light of the similarity between $\langle 211 \rangle$ and $\langle 210 \rangle$ bonds.

Let us now consider a model based on the possibility of a growth-induced preferential site occupation in the dodecahedral sublattice. We find that there are twelve different rare-earth sites defined with respect to the NNT, NNO, and NNNT ions. Of these twelve sites only six are magnetically inequivalent. These twelve sites can be divided into three subsets of four sites each with respect to the NNT ions alone. In Table I we list all of the $\langle 100 \rangle$, $\langle 210 \rangle$, and $\langle 211 \rangle$ bonds of the four sites belonging to the X subset. We note that sites $\bar{X}_1$ and $\bar{X}_2$ are derived from X_1 and X_2 by reflecting all neighbors in the y-z plane. Also site X_2 is derived from site X_1 by reflecting only the NNNT neighbors in the x-y plane. One can construct similar tables for the $(Y_1, \bar{Y}_1, Y_2, \bar{Y}_2)$ and $(Z_1, \bar{Z}_1, Z_2, \bar{Z}_2)$ subsets by cyclically permuting all the neighbors for each X site of Table I. Defining the site preference of the A ion by η_{X_1}, $\eta_{\bar{X}_1}$, η_{X_2}, $\eta_{\bar{X}_2}$, and so on, and considering, as in the pair-preference model,[2,3] that the rare-earth–iron magnetic interaction[6] is dipolar in the first order, we can define the magnetic anisotropy for the A ion at the ith site as

$$E_i{}^s = N_A\eta_i\left[\sum_{j=1}^{2} l_{AC}{}^{\mathrm{I}}(\cos^2\varphi_{ij} - \tfrac{1}{3}) + \sum_{k=1}^{4} l_{AC}{}^{\mathrm{II}}(\cos^2\varphi_{ik} - \tfrac{1}{3}) + \sum_{n=1}^{4} l_{AC}{}^{\mathrm{III}}(\cos^2\varphi_{in} - \tfrac{1}{3})\right], \tag{3}$$

where $l_{AC}{}^{\mathrm{I}}$, $l_{AC}{}^{\mathrm{II}}$, and $l_{AC}{}^{\mathrm{III}}$ designate the pair interactions between A and the NNT, NNO, and NNNT ions, respectively. The angles between the various bonds at the ith site and the magnetization are denoted by the φ_{ij}, φ_{ik}, and φ_{in}. The number of A ions per unit volume is given by N_A. Using Eq. (3) and Table I we then find that the total site anisotropy in the $\{100\}$ coordinate system is given by

$$E^s = N_A l_0(\eta_X{}'\alpha_x{}^2 + \eta_Y{}'\alpha_y{}^2 + \eta_Z{}'\alpha_z{}^2) + \tfrac{8}{3}l_{AC}{}^{\mathrm{III}}[\eta_X{}''\alpha_y\alpha_z + \eta_Y{}''\alpha_x\alpha_z + \eta_Z{}''\alpha_x\alpha_y], \tag{4}$$

Table I. The four sites of the X subset, the bonds to the neighboring iron ions, and the site- and bond-preference parameters.

Site	Site Preference	N.N.T. Bond	N.N.T. Bond Preference (110)	N.N.T. Bond Preference (112)	N.N.O. Bond	N.N.O. Bond Preference (110)	N.N.O. Bond Preference (112)	N.N.N.T. Bond	N.N.N.T. Bond Preference (110)	N.N.N.T. Bond Preference (112)
X_1	η_{X_1}	[100]	ϵ_1^I	ϵ_1^I	[120]	ϵ_3^{II}	ϵ_3^{II}	[112]	ϵ_2^{III}	ϵ_6^{III}
		[$\bar{1}$00]	ϵ_1^I	ϵ_1^I	[1$\bar{2}$0]	ϵ_1^{II}	ϵ_1^{II}	[1$\bar{1}$2]	ϵ_0^{III}	ϵ_4^{III}
					[$\bar{1}$02]	ϵ_1^{II}	ϵ_3^{II}	[$\bar{1}$21]	ϵ_1^{III}	ϵ_3^{III}
					[$\bar{1}$0$\bar{2}$]	ϵ_1^{II}	ϵ_5^{II}	[$\bar{1}$2$\bar{1}$]	ϵ_3^{III}	ϵ_5^{III}
$\bar{X}_1$	$\eta_{\bar{X}_1}$	[$\bar{1}$00]	ϵ_1^I	ϵ_1^I	[$\bar{1}$20]	ϵ_1^{II}	ϵ_1^{II}	[$\bar{1}$12]	ϵ_0^{III}	ϵ_4^{III}
		[100]	ϵ_1^I	ϵ_1^I	[1$\bar{2}$0]	ϵ_3^{II}	ϵ_3^{II}	[$\bar{1}$$\bar{1}$2]	ϵ_2^{III}	ϵ_6^{III}
					[102]	ϵ_1^{II}	ϵ_5^{II}	[121]	ϵ_3^{III}	ϵ_5^{III}
					[10$\bar{2}$]	ϵ_1^{II}	ϵ_3^{II}	[12$\bar{1}$]	ϵ_1^{III}	ϵ_3^{III}
X_2	η_{X_2}	[100]	ϵ_1^I	ϵ_1^I	[120]	ϵ_3^{II}	ϵ_3^{II}	[11$\bar{2}$]	ϵ_2^{III}	ϵ_2^{III}
		[$\bar{1}$00]	ϵ_1^I	ϵ_1^I	[1$\bar{2}$0]	ϵ_1^{II}	ϵ_1^{II}	[1$\bar{1}$2]	ϵ_0^{III}	ϵ_4^{III}
					[$\bar{1}$02]	ϵ_1^{II}	ϵ_3^{II}	[$\bar{1}$2$\bar{1}$]	ϵ_1^{III}	ϵ_1^{III}
					[$\bar{1}$0$\bar{2}$]	ϵ_1^{II}	ϵ_5^{II}	[$\bar{1}$21]	ϵ_3^{III}	ϵ_1^{III}
$\bar{X}_2$	$\eta_{\bar{X}_2}$	[$\bar{1}$00]	ϵ_1^I	ϵ_1^I	[$\bar{1}$20]	ϵ_1^{II}	ϵ_1^{II}	[$\bar{1}$1$\bar{2}$]	ϵ_0^{III}	ϵ_4^{III}
		[100]	ϵ_1^I	ϵ_1^I	[1$\bar{2}$0]	ϵ_3^{II}	ϵ_3^{II}	[$\bar{1}$$\bar{1}$2]	ϵ_2^{III}	ϵ_2^{III}
					[102]	ϵ_1^{II}	ϵ_5^{II}	[12$\bar{1}$]	ϵ_3^{III}	ϵ_1^{III}
					[10$\bar{2}$]	ϵ_1^{II}	ϵ_3^{II}	[1$\bar{2}$1]	ϵ_1^{III}	ϵ_1^{III}

where

$$l_0 = 2l_{AC}{}^I - \tfrac{4}{5}l_{AC}{}^{II} - l_{AC}{}^{III};$$

$\eta_X' = \eta_{X_1} + \eta_{\bar{X}_1} + \eta_{X_2} + \eta_{\bar{X}_2}$, similarly for η_Y' and η_Z';

$\eta_X'' = \eta_{X_1} + \eta_{\bar{X}_1} - \eta_{X_2} - \eta_{\bar{X}_2}$, similarly for η_Y'' and η_Z''.

If, as in the pair preference model, we assume that the site preference of ion A is determined by the growth facet, then we may use our knowledge of the pair-preference parameters to establish the main features of the site-preference parameters. Thus, the site preference η_i can be related to the pair preferences of the bonds appropriate to site i by

$$\eta_i = m^I \sum_{j=1}^{2} \epsilon_{(ij)}{}^I + m^{II} \sum_{k=1}^{4} \epsilon_{(ik)}{}^{II} + m^{III} \sum_{l=1}^{4} \epsilon_{(il)}{}^{III}, \qquad (5)$$

where m^I, m^{II}, and m^{III} are weighting factors for the different bond classes, and $\epsilon_i{}^{I,II,III}$ are the appropriate pair-preference parameters for the ith site. Without knowing the weighting factors, one can still determine the general relationships between the various η_i's by use of Table I where all of the pair-preference parameters for the X sites are listed for both the (110) and (112) facets.

If we consider only NNT and NNO ions, it is clear from Table I that for both the (110) and (112)

facets,

$$\eta_{X_1} = \eta_{\overline{X}_1} = \eta_{X_2} = \eta_{\overline{X}_2} = \eta_{Y_1} = \eta_{\overline{Y}_1} = \eta_{Y_2} = \eta_{\overline{Y}_2},$$ (6a)

$$\eta_{Z_1} = \eta_{\overline{Z}_1} = \eta_{Z_2} = \eta_{\overline{Z}_2}.$$ (6b)

In the $\{100\}$ coordinate system, the site anisotropies under both the (110) and (112) facets are given by Eq. (4) as

$$E_{(110)}{}^s = E_{(112)}{}^s = 4N_A l_0 (\eta_{Z_1} - \eta_{X_1}) \alpha_z{}^2 + C_3.$$ (7)

We thus have a simple uniaxial anisotropy under both facets, a prediction not supported by the experimental data.[2,3] If we now include the NNNT ions, we find from Table I that for the (110) facet Eq. (6a) is still valid but (6b) now becomes

$$\eta_{Z_1} = \eta_{\overline{Z}_1}; \quad \eta_{Z_2} = \eta_{\overline{Z}_2}.$$ (8)

Equation (4) then gives

$$E_{(110)}{}^s = 2N_A l_0 (\eta_{Z_1} + \eta_{Z_2} - 2\eta_{X_1}) \alpha_z{}^2 + \tfrac{16}{3} N_A l_{AC}{}^{III} (\eta_{Z_1} - \eta_{Z_2}) \alpha_x \alpha_y + C_4.$$ (9)

Transforming to the $\{110\}$-coordinate system where $x \equiv [001]$, $y \equiv [1\overline{1}0]$, and $z \equiv [110]$, we have

$$E_{(110)}{}^s = 2N_A l_0 (\eta_{Z_1} + \eta_{Z_2} - 2\eta_{X_1}) \alpha_x{}^2 + \tfrac{8}{3} N_A l_{AC}{}^{III} (\eta_{Z_1} - \eta_{Z_2})(\alpha_z{}^2 - \alpha_y{}^2) + C_4.$$ (10)

Equation (10) depicts the same type of orthorhombic anisotropy as that found for the pair-preference model in Eq. (1).

For the (112) facet we now find that Eq. (8) is valid but Eq. (6a) becomes

$$\eta_{X_1} = \eta_{\overline{X}_1} = \eta_{Y_1} = \eta_{\overline{Y}_1}; \quad \eta_{X_2} = \eta_{\overline{X}_2} = \eta_{Y_2} = \eta_{\overline{Y}_2}.$$ (11)

The site anisotropy under the (112) facet in the $\{100\}$-coordinate system is given by Eq. (4) as

$$E_{(112)}{}^s = 2N_A l_0 [(\eta_{X_1} + \eta_{X_2})(\alpha_x{}^2 + \alpha_y{}^2) + (\eta_{Z_1} + \eta_{Z_2}) \alpha_z{}^2] + \tfrac{8}{3} N_A l_{AC}{}^{III} [2(\eta_{X_1} - \eta_{X_2}) \alpha_z (\alpha_x + \alpha_y) + (\eta_{Z_1} - \eta_{Z_2}) \alpha_x \alpha_y].$$ (12)

Transforming to the $\{112\}$-coordinate system where $x \equiv [11\overline{1}]$, $y \equiv [\overline{1}10]$, and $z \equiv [112]$, we have

$$E_{(112)}{}^s = 2N_A l_0 [(\eta_{X_1} + \eta_{X_2})(\tfrac{2}{3} \alpha_x{}^2 + \alpha_y{}^2 + \tfrac{1}{3} \alpha_z{}^2 + \tfrac{2}{3}\sqrt{2} \alpha_x \alpha_z) + (\eta_{Z_1} + \eta_{Z_2})(\tfrac{1}{3} \alpha_x{}^2 + \tfrac{2}{3} \alpha_z{}^2 - \tfrac{2}{3}\sqrt{2} \alpha_x \alpha_z)]$$

$$+ N_A l_{AC}{}^{III} [\eta_{Z_1} - \eta_{Z_2})(\tfrac{1}{3}\alpha_z{}^2 - \tfrac{1}{2}\alpha_y{}^2 + \tfrac{1}{6}\alpha_z{}^2 + \tfrac{1}{3}\sqrt{2}\alpha_x \alpha_z) - 2(\eta_{X_1} - \eta_{X_2})(\tfrac{2}{3}\alpha_x{}^2 - \tfrac{2}{3}\alpha_z{}^2 - \tfrac{1}{3}\sqrt{2}\alpha_x \alpha_z)].$$ (13)

Equation (13) depicts the same type of orthorhombic anisotropy as that found for the pair-preference model in Eq. (2).

The symmetries of the noncubic anisotropies observed in these flux-grown garnets can thus be explained equally well in terms of either a pair-preference model or a site preference model. Since both models depend on the facet normal, it is clear that the predicted anisotropy symmetries must be consistent with the facet symmetries, and so they are. Unlike the pair-preference model, the site-preference model will predict a uniaxial anisotropy if only NNT and NNO ions are considered. Inclusion of the NNNT ions results in the proper orthorhombic anisotropy from the site model. Inclusion of these neighbors is not unreasonable in light of the relative strength of their superexchange interaction to the rare-earth ions. Finally, we would like to remark that the philosophical distinction between the two models resides primarily in the interpretation of the crystallization process. In the pair-preference model, we assume that clusters of rare-earth and iron cations crystallize at the facet surface *simultaneously*, and to a first approximation as rare-earth–iron pairs defined by the pair-preference parameters ϵ_i. In the site-preference model, the assumption is that the rare-earth ions crystallize *after* the iron ions have already solidified and defined the environment and the site-preference parameters η_i. The difference between the site- and pair-bond models at crystallization is also reflected in the calculation of the bulk anisotropy; namely, that the preferred pair directions at the time of crystallization also appear in the calculation of the bulk anisotropy (perhaps through local distortions associated with this preferential pairing, which in turn affect the various pair interactions anisotropically). For this reason the pair model predicts an orthorhombic anisotropy when only the NNT and NNO ions are considered, while the site model predicts a uniaxial anisotropy.

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Dispersion Effect in the Iwamoto-Yamada Cluster Expansion*

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The use of auxiliary single-particle potentials permits the inclusion of the dispersion effect in the energy of a many-Fermion system calculated in the independent-pair approximation of the Iwamoto-Yamada cluster expansion.

In a previous paper,[1] it is pointed out that the usual Iwamoto-Yamada (IY) cluster expansion[2] for the energy per particle of a system of fermions in the independent-pair approximation does not contain the dispersion effect[1,3] of the nuclear medium which already appears in the independent-pair approximation of the Brueckner-Bethe-Goldstone reaction-matrix theory with self-consistent single-particle energies.

The IY cluster energy in the independent-pair approximation can be written as

$$E/N \approx N^{-1}\sum_i \langle i|t_1|i\rangle + \tfrac{1}{2}N^{-1}\sum_{ij}\langle ij|\Omega^\dagger v_{12}\Omega + \Omega^\dagger(t_1 + t_2)\Omega - \Omega^\dagger\Omega(t_1 + t_2)|ij-ji\rangle = \epsilon_1 + \epsilon_2, \tag{1}$$

where t_1 is the single-particle kinetic-energy operator, v_{12} is the two-body interaction, and Ω is a pair correlation operator—a generalization of the Jastrow correlation function $f(r_{ij})$. The corresponding reaction-matrix energy is $W_1 + W_2(\overline{U}_p)$, where $W_1 = \epsilon_1 = N^{-1}\sum_i \langle i|t_1|i\rangle$ and $W_2(\overline{U}_p) = \tfrac{1}{2}N^{-1}\sum_{ij}\langle ij|G(\overline{U}_p)|ij-ji\rangle$. The reaction matrix

$$G(\overline{U}_p) = v - v[Q/e(\overline{U}_p)]G(\overline{U}_p)$$

appearing in W_2 is often calculated with

$$e(\overline{U}_p) = t_1 + t_2 + 2\overline{U}_p - (\epsilon_1 + \epsilon_2),$$

i.e., a constant single-particle potential $\overline{U}_p$ in intermediate states and self-consistent single-particle energies ϵ_i in occupied states. The projection operator Q in the reaction-matrix equation ensures that both particles in intermediate states are outside the Fermi sea.

If the correlation operator Ω in Eq. (1) is taken to be the reaction-matrix correlation operator $\Omega = 1 - (Q/e)G$, the pair contribution to the cluster energy can be expressed roughly as[1]

$$\epsilon_2 \approx (1 + 2\kappa)W_2(\overline{U}_p) - \kappa\overline{U}_p, \tag{2}$$

where

$$\kappa = \frac{1}{N}\sum_{ij}\left\langle ij\left|G\frac{Q}{e}\frac{Q}{e}G\right|ij-ji\right\rangle$$

is the single-particle excitation probability due to independent-pair correlations. Thus the two theories give different energies in the independent-pair approximation. The absence of the dispersion term $\kappa[\overline{U}_p - 2W_2(\overline{U}_p)]$ in the cluster energy ϵ_2 has an effect not only in worsening the saturation properties of the system,[1,3] but also in the inability to prevent the pair correlation from becoming unrealistically large[1] in the original variational approach of the IY cluster expansion.[2]

We would like to point out in this paper that this dispersion effect can be made to appear in the independent-pair approximation of the cluster expansion if the Hamiltonian

$$H = \sum_\alpha t_\alpha + \tfrac{1}{2}\sum_{\alpha\beta} v_{\alpha\beta} \tag{3}$$

is written in the familiar form

$$H = \sum_\alpha h_\alpha + \tfrac{1}{2}\sum_{\alpha\beta} v_{\alpha\beta}', \tag{4}$$