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**OGUCHI YAKLAŞIMINDA KARMA SPİN-2 VE SPİN-1/2 ANİZOTROPİK
HEISENBERG MODELİNİN FAZ DİYAGRAMLARI**

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ÖZET

Bu projede, karma spin-2 ve spin-1/2 Hesienberg modelinde deęiş-tokuş enerjisi ve kristal alan etkileri Oguchi yaklaşımı kullanılarak kare ve basit kübik kafes üzerinde çalışılmıştır. Düzen parametrelerinin, manyetik dipol ve kuadrupol moment, ve serbest enerjinin sıcaklıkla olan deęişimleri incelenerek sistemin mümkün olan düzlemlerdeki faz diyagramları elde edilmiştir. Detaylı faz diyagramları (D/J , $k_B T/J$) ve (Δ , $k_B T/J$) düzlemlerinde sırasıyla verilen Δ ve D/J deęerleri için elde edilmiştir. Elde edilen faz diyagramlarında kararlı ya da kararsız olsun bütün çözümler gösterilmiştir. Modelin üçlü kritik ve izole edilmiş kritik noktaların yanı sıra ikinci- ve birinci seviye faz geçişleri verdiği bulunmuştur. Model aynı zamanda verilmiş sistem parametreleri için iki telafi (compensation) sıcaklığı vermiştir ki buda reentrant olayına sebebiyet vermiştir. Modelin düşük sıcaklık bölgesindeki davranışı çok karmaşıktır ki bundan dolayı bu modelin güvenilirliğinin tespiti için daha ileri seviyede incelenmesi gereklidir.

Anahtar Kelimeler: Heisenberg Modeli; Oguchi Yaklaşımı; Deęiş-Tokuş Anizotropisi; Kristal Alan; Karma Spin.

ABSTRACT

In this project, the mixed spin-2 and spin-1/2 Heisenberg model was studied on square and simple cubic lattices by using the Oguchi approximation to examine the effects of exchange anisotropy and crystal field. The thermal variations order-parameters, i.e. magnetization and quadrupole moment, and free energy were investigated to obtain the possible phase diagrams of the model. The detailed phase diagrams were obtained on the (D/J , $k_B T/J$) and (Δ , $k_B T/J$) planes for given values of Δ and D/J , respectively. In the phase diagrams all possible solutions were illustrated whether stable or not. The model has yielded the second and first-order phase transitions, in addition to the tricritical and isolated critical points. The model has also given two compensation temperatures for given system parameters, therefore, they exhibit reentrant behavior. It was found that the low temperature behavior of the model is very complicated, therefore, the reliability of the Oguchi approximation should be investigated further.

Keywords: Mixed Spin; Heisenberg Model; Oguchi Approximation; Exchange Anisotropy; Crystal Field, Mixed Spin.

1- GENEL BİLGİLER ve TEORİ

Literatürde tek-tip spin sistemlerin incelenmesinden sonraki mantıklı yaklaşım bu spinleri farklı tipteki spinlerle farklı yapıları oluşturacak şekilde karıştırarak elde edilecek olan karma spin sistemlerini incelemektir. Karma spin sistemlerinin çalışılması telafi sıcaklığı adı verilen önemli bir fiziksel olayın bulunmasına vesile olmuştur ki buda teknoloji ve sanayide birçok çalışma alanı bulmuştur. Buna ilaveten bu karma spin sistemlerinde elde edilen faz diyagramları daha zengin hale gelmektedir ki bundan dolayı bu sistem daha fazla ilgi çekmektedir. Ising modelinde spinler z-ekseni olarak seçilen tek bir doğrultuda yönelebilirler. Bu sınırlama ortadan kaldırıldığında, yani spinlere üç-boyutlu uzayda istedikleri yönde yönelebilmeye imkanı verildiğinde, bu kuantum mekaniksel olan sistemlere sebebiyet verir ki bu sistemler de Heisenberg modeli olarak adlandırılır. Bu model de spin operatörleri birbirleri ile sıra değiştirmezler bundan dolayı da fiziksel gözlenebilirlerin ölçülmesinde bazı belirsizlikler ortaya çıkar. Bu sebeple bu tip problemin çözümünde kesin çözümlerin elde edilmesi mümkün değildir, dolayısıyla çözüm elde etmek için bir takım yaklaşımlar gerekir ki bu yaklaşımlar da genellikle modelin niteliksel tasvirini bir şekilde verse de eksiklikleri mevcuttur. Bu amaçla bu projede kare ve basit kübik kafes üzerinde karma spin-2 ve spin-1/2 Heisenberg ferrimanyetik sistemini Oguchi yaklaşımını (OA) kullanarak çalıştık. Heisenberg modelinde OA tek tip veya karma spin sistemleri için daha önce kullanılmış olup ilginç sonuçlar elde edilmiştir. Bu çalışmalardan bazıları aşağıda verilmiştir. Dzyaloshinsky-Moriya etkileşimini dahil eden spin-1/2 anizotropik Heisenberg modelinin termodinamik özellikleri [1], yine spin-1/2 sisteminin ikinci en-yakın komşu spinleri de dikkate alınarak sistemin manyetizasyonu, iç enerjisi, ısı kapasitesi, entropisi ve serbest enerjisi [2] çalışılmıştır. Karma spin-1 ve spin-1/2 sisteminde değiş-tokuş etkileşme parametresi ve tek-spin anizotropisinin etkileri [3], telafi sıcaklığı [4] ve manyetik alınganlık [5] çalışılmıştır. Benzer fiziksel özellikler karma spin-3/2 ve spin-1/2 sisteminde de ele alınmıştır [6]. Bu tip çalışmalarda sadece basit kübik kafes yapısı ele alınmıştır çünkü Mermin-Wagner teoremi $d \leq 2$ boyutunda yeterince kısa-mesafeli etkileşimler için sürekli simetrilerin sonlu sıcaklıklarda kendiliğinden kırılmayacağını ifade eder [7]. Dolayısı ile OA yaklaşımı düzlemsel izotropik Heisenberg modeli için Mermin-Wagner teoremi ile uyum içerisinde değildir. Bu projede Mermin-Wagner teoremine zıt düşmemek için her ne kadar basit kübik yapıya karşılık gelen $z=6$ en-yakın komşu spinli yapı ele alınmış olsa da kare

kafes için $z=4$ yapısı da aynı titizlikle çalışarak Mermin-Wagner teoremi test edilmeye çalışılmıştır. Literatür taraması bize karma spin-2 ve spin-1/2 sisteminin çoğunlukla Ising modelinde çalışıldığını göstermektedir. Bu sistemin düzen parametrelerinin termal davranışları ve faz diyagramları koordinasyon sayıları $z=3, 4, 5$ ve 6 için Bethe kafesi üzerinde en-yakın komşu etkileşimler ele alınarak Blume-Capel modelinde kesin tekrarlamalı bağıntıları terimlerinde çalışılmıştır [8]. Spin değerleri $\sigma (\pm 1/2)$ ve $S (\pm 2, \pm 1, 0)$ olan karma spin sisteminin kritik davranışları çalışılıp Monte-Carlo simülasyonu kullanılarak kesin taban durumu hesaplamaları yapılarak modelin sonlu-sıcaklık faz diyagramları elde edilmiştir [9]. Ferromanyetik elmas zincirinin manyetik özellikleri Ising modelinde Monte-Carlo ve etkin-alan teorisi kullanılarak çalışılmıştır [10]. Heisenberg modeli ile yapılan tek çalışma Heisenberg spinlerinin kuantumsal yapısını da dahil eden iki-zamanlı Green fonksiyonu tekniği ile kare kafes üzerinde sistemin telafi sıcaklığı ve kritik davranışlarını ele alan çalışmadır [11]. Bu çalışmalarda genel olarak kristal alan etkileri ele alınmıştır fakat üç-boyutlu durumda spinler bir doğrultuda diğer doğrultulara göre daha kuvvetli bir etkileşme sergileyebilirler dolayısı ile değiş-tokuş anizotropisinin faz diyagramlarına olan etkisini çalışmak ilginçtir ki bu projede bu etki de detaylı bir şekilde çalışılmıştır.

Karma spin-2 ve spin-1/2 içeren çok fazla deneysel çalışma mevcut olmasa da bu karma spin sistemini inceleyen iki çalışma mevcuttur: eşit olmayan kuantum spinlerini içeren makro-halkalı $S=2$ ve çapraz-bağlı radikaller $S=1/2$ sahip polimer [12] ve $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ makro-halka üzerindeki öz ısı çalışmaları [13].

Bu projede, karma spin-2 ve spin-1/2 Heisenberg modelinde değiş-tokuş anizotropisi ve kristal alanın etkileri OA yaklaşımında kare ve basit kübik kafesler üzerinde incelenmiştir. Sistemin detaylı faz diyagramları $(D/J, k_B T/J)$ ve $(\Delta, k_B T/J)$ düzlemlerinde sırasıyla verilen Δ ve D/J değerleri için düzen parametrelerinin sıcaklığa göre değişimleri incelenerek elde edilmiştir. Sistemin sergilediği faz geçişleri ve bunlara ait faz çizgilerinin yanı sıra özel kritik noktalarda detaylıca çalışılmış ve telafi sıcaklık çizgileri de elde edilmiştir.

2- FORMÜLASYON

Bu projede karma spin- S_A ve spin- S_B Hamiltoniyeni

$$\mathcal{H} = -J \sum_{\langle ij \rangle} [(1 - \Delta)(\hat{S}_{iA}^x \hat{S}_{jB}^x + \hat{S}_{iA}^y \hat{S}_{jB}^y) + \hat{S}_{iA}^z \hat{S}_{jB}^z] - D \sum_{i \in A} (\hat{S}_{iA}^z)^2,$$

şeklinde alınmış olup burada $\delta = x, y, z$ olmak üzere S_{iA}^δ ve S_{jB}^δ sırasıyla spin-2'li A ve spin-1/2'li B alt örgülerine ait operatörlerin bileşenleridir. J en yakın komşu spinler arasındaki bilineer değiş-tokuş etkileşim parametresi, D sadece spin-2 konumlarında etkin olan kristal alan, Δ değiş-tokuş anizotropi parametresi olup $0 \leq \Delta \leq 1$ şartını sağlar.

Oguchi yaklaşımında, en yakın komşu spin çiftleri arasındaki etkileşimler kesin olarak hesaplanırken spinler arasındaki geri kalan etkileşimler ortalama-alan etkileşimlerinde de genel olarak yapıldığı gibi bir etkin alan terimi ile değiştirilecektir. Bundan dolayı, etkin Oguchi Hamiltonyeni

$$\mathcal{H}_{ij} = -J[(1 - \Delta)(\hat{S}_{iA}^x \hat{S}_{jB}^x + \hat{S}_{iA}^y \hat{S}_{jB}^y) + \hat{S}_{iA}^z \hat{S}_{jB}^z] - D(\hat{S}_{iA}^z)^2 - h_i \hat{S}_{iA}^z + h_j \hat{S}_{jB}^z$$

şeklinde alınır ki burada ortalama-alan terimleri

$$h_i = (z - 1)JM_B$$

$$h_j = (z - 1)JM_A$$

olup

$$M_A = \langle \hat{S}_{iA}^z \rangle$$

$$M_B = \langle \hat{S}_{jB}^z \rangle$$

sırasıyla alt örgülere ait manyetizasyonlar, z en yakın komşu spinlerin sayısı ve $\langle \dots \rangle$ termal ortalamaya karşılık gelir.

Oguchi yaklaşımında Heisenberg modelinde gerekli termodinamik fonksiyonlara ait formülasyonu elde etmek için

$$\mathcal{H}_{ij} | n \rangle = E_n | n \rangle, \quad n = 1, 2, \dots, 10$$

şeklindeki özdeğer denklemi çözülmelidir ki burada $|n\rangle$ özvektörler ve E_n bunlara karşılık gelen özvektörlerdir. Bu amaçla bu özvektörleri hesaplamada kullanılacak olan mümkün taban vektörlerini elde etmekte spin-2 için $|S_A, m_{S_A}\rangle_i$ ve spin-1/2 için $|S_B, m_{S_B}\rangle_j$ vektörlerinin $|S_A, m_{S_A}\rangle_i \otimes |S_B, m_{S_B}\rangle_j$ şeklindeki direkt çarpımları kullanılacaktır ki bunlar

$$\begin{aligned} |I\rangle &= |2, 2\rangle_i |1/2, 1/2\rangle_j, & |II\rangle &= |2, 2\rangle_i |1/2, -1/2\rangle_j, \\ |III\rangle &= |2, 1\rangle_i |1/2, 1/2\rangle_j, & |IV\rangle &= |2, 1\rangle_i |1/2, -1/2\rangle_j, \\ |V\rangle &= |2, 0\rangle_i |1/2, 1/2\rangle_j, & |VI\rangle &= |2, 0\rangle_i |1/2, -1/2\rangle_j, \\ |VII\rangle &= |2, -1\rangle_i |1/2, 1/2\rangle_j, & |VIII\rangle &= |2, -1\rangle_i |1/2, -1/2\rangle_j, \\ |IX\rangle &= |2, -2\rangle_i |1/2, 1/2\rangle_j, & |X\rangle &= |2, -2\rangle_i |1/2, -1/2\rangle_j \end{aligned}$$

şeklinde. Bu taban vektörler takımı kullanılarak Oguchi Hamiltonyeninin özdeğer ve özvektörlerini elde etmekte kullanılacak olan 10×10 matris elde edilmiştir. Elde edilen matrisin elemanları $i, j = 1, 2, 3, \dots, 10$ olmak üzere $\langle i | E_{ij} | j \rangle$ şeklinde olup sıfırdan farklı elemanları

$$\begin{aligned} E_{11} &= -J - 4D - 2h_i - h_j/2, & E_{22} &= J - 4D - 2h_i + h_j/2, \\ E_{33} &= -J/2 - D - h_i - h_j/2, & E_{44} &= J/2 - D - h_i + h_j/2, \\ E_{55} &= -h_j/2, & E_{66} &= h_j/2, \\ E_{77} &= J/2 - D + h_i - h_j/2, & E_{88} &= -J/2 - D + h_i + h_j/2, \\ E_{99} &= J - 4D + 2h_i - h_j/2, & E_{1010} &= -J - 4D + 2h_i + h_j/2, \\ E_{23} &= E_{32} = -J(1 - \Delta), & E_{45} &= E_{54} = -\sqrt{6}J(1 - \Delta)/2, \\ E_{67} &= E_{76} = -\sqrt{6}J(1 - \Delta)/2, & E_{89} &= E_{98} = -J(1 - \Delta). \end{aligned}$$

olarak elde edilmiştir. Bu tabanlarda elde edilen Oguchi Hamiltonyeninin matris gösteriminin simetrik olduğu aşıkardır. Son basamak olarak bu matrisin özdeğer ve özvektörleri bulunmuştur. Buradaki amacımız için özdeğerlerin hesaplanması yeterlidir. Dolayısı ile hesapladığımız 10 özdeğer

$$\begin{aligned} E_{1,2} &= -4D \pm 2h_i \pm h_j/2 - J, \\ E_{3,4} &= [-10D + 6h_i + J \pm [36D^2 - 24Dh_i + 4h_i^2 + 24Dh_j - 8h_ih_j + 4h_j^2 - 36DJ \\ &\quad + 12h_ij - 12h_j^2 + 9J^2 + 64J^2]^{1/2}]/4, \\ E_{5,6} &= [-10D - 6h_i + J \pm [36D^2 + 24Dh_i + 4h_i^2 - 24Dh_j - 8h_ih_j + 4h_j^2 - 36DJ \\ &\quad - 12h_ij + 12h_j^2 + 9J^2 + 64J^2]^{1/2}]/4, \\ E_{7,8} &= [-4D - 4h_i + 2J \pm [(4D + 4h_i - 2J)^2 - 16(2Dh_j + 2h_ih_j - h_j^2 - h_ij - 24J^2)]^{1/2}]/8, \\ E_{9,10} &= [-4D + 4h_i + 2J \pm [(4D - 4h_i - 2J)^2 - 16(-2Dh_j + 2h_ih_j - h_j^2 + h_ij - 24J^2)]^{1/2}]/8 \end{aligned}$$

şeklinde olup burada $J'=J/2(1-\Delta)$ 'dır. Elde edilen özdeğerler kullanılarak sistemin bütün termodinamik fonksiyonlarını elde etmede kullanabileceğimiz bölüşüm fonksiyonu ise

$$Z = \sum_{i=1}^n e^{\lambda_i}, n=10$$

ile verilir ki burada $\lambda_i = E_i$ 'dir. A alt örgülü spin-2 için sistemin düzen parametreleri manyetizasyon ve kuadrupol moment olup, M_A ve Q_A , sırasıyla

$$M_A = \frac{1}{\beta Z} \frac{\partial Z}{\partial h_i} \quad \text{ve} \quad Q_A = \frac{1}{\beta Z} \frac{\partial Z}{\partial D}$$

ifadelerinden hesaplanırken B alt örgülü spin-1/2 sistemi için tek düzen parametresi olan manyetizasyon

$$M_B = \frac{1}{\beta Z} \frac{\partial Z}{\partial h_j}$$

ifadesinden hesaplanacaktır, burada $\beta = 1/(k_B T)$ 'dir. Sistemin çözümlerinin yapısına, kararlı veya kararsız vs..., olduğuna karar vermede kullanılacak olan serbest enerji ifadesi ise

$$F(T, M_A, M_B) = -kT \ln Z + J(z-1)M_A M_B$$

şeklindedir. Ortalama ve manyetizasyonlar farkı ise

$$M_T = (M_A + M_B)/2 \quad \text{ve} \quad M_C = |M_A - M_B|$$

ile verilir. Burada eğer sistem telafi sıcaklığı verirse bu sıcaklıkta M_C 'nin sıfır olduğu aşıkardır ki bu durum kısaca alt kafes manyetizasyonlarının telafi sıcaklığında eşit oldukları anlamına gelir:

$$|M_A(T_{comp})| = |M_B(T_{comp})|$$

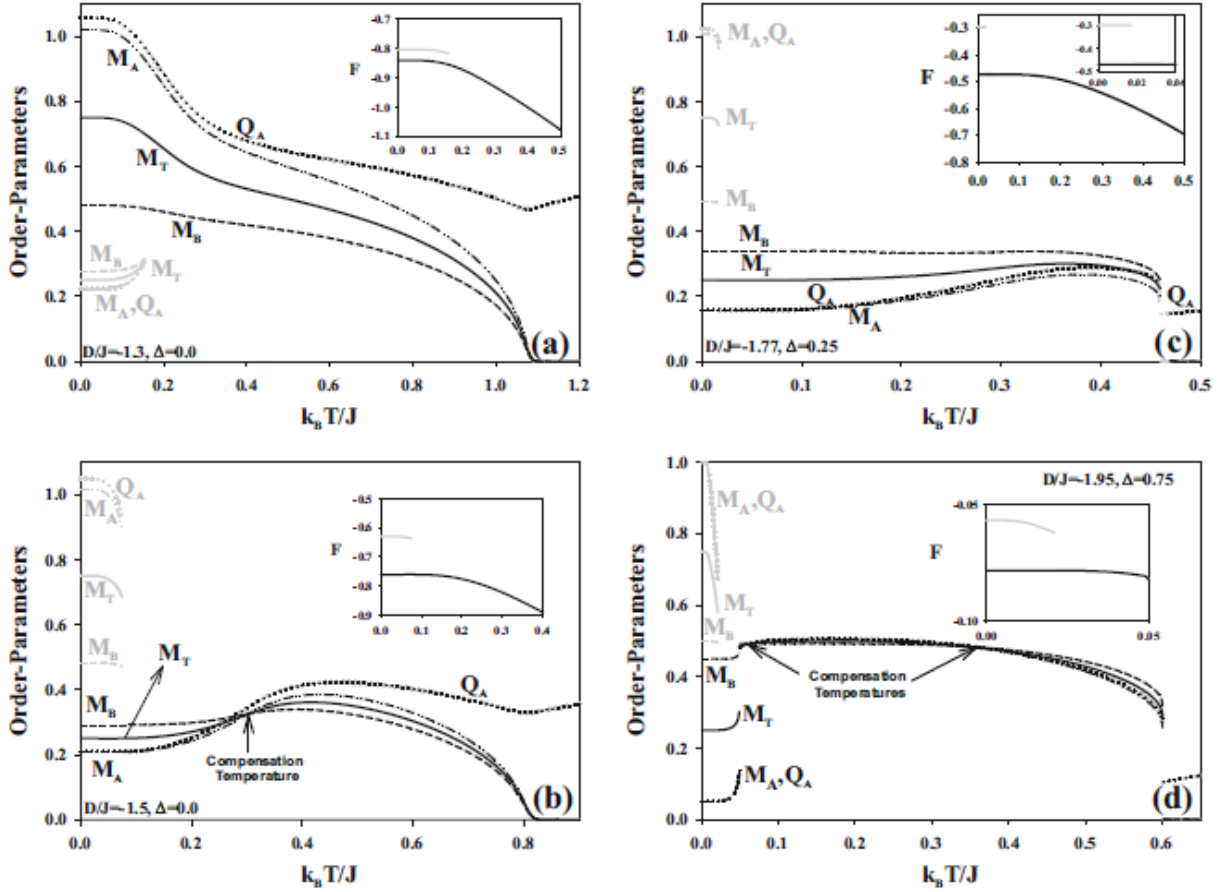
Bütün bu formülasyonlardan sonra sistemin faz diyagramları (D/J , $k_B T/J$) ve (Δ , $k_B T/J$) düzlemlerinde sırasıyla verilen Δ ve D/J değerleri elde edilmiştir. Bu faz diyagramında karma spin-2 ve spin-1/2 sisteminin sergileyebileceği ikinci- ve birinci seviye faz geçiş sıcaklıkları sistemin düzen parametrelerinin sıcaklıkla değişimleri incelenip detaylı olarak elde edilmiştir. Bunun yanı sıra sistemin verebileceği telafi sıcaklıkları da detaylı olarak ele alınmıştır.

3- FAZ DİYAGRAMLARI ve SONUÇLAR

Faz diyagramlarını vermeden önce düzen parametreleri ikinci- veya birinci-seviye faz geçişi sergilediğinde sıcaklıkla değişimlerini hem kare ($z=4$) ve hem de basit kübik kafes ($z=6$) için verelim.

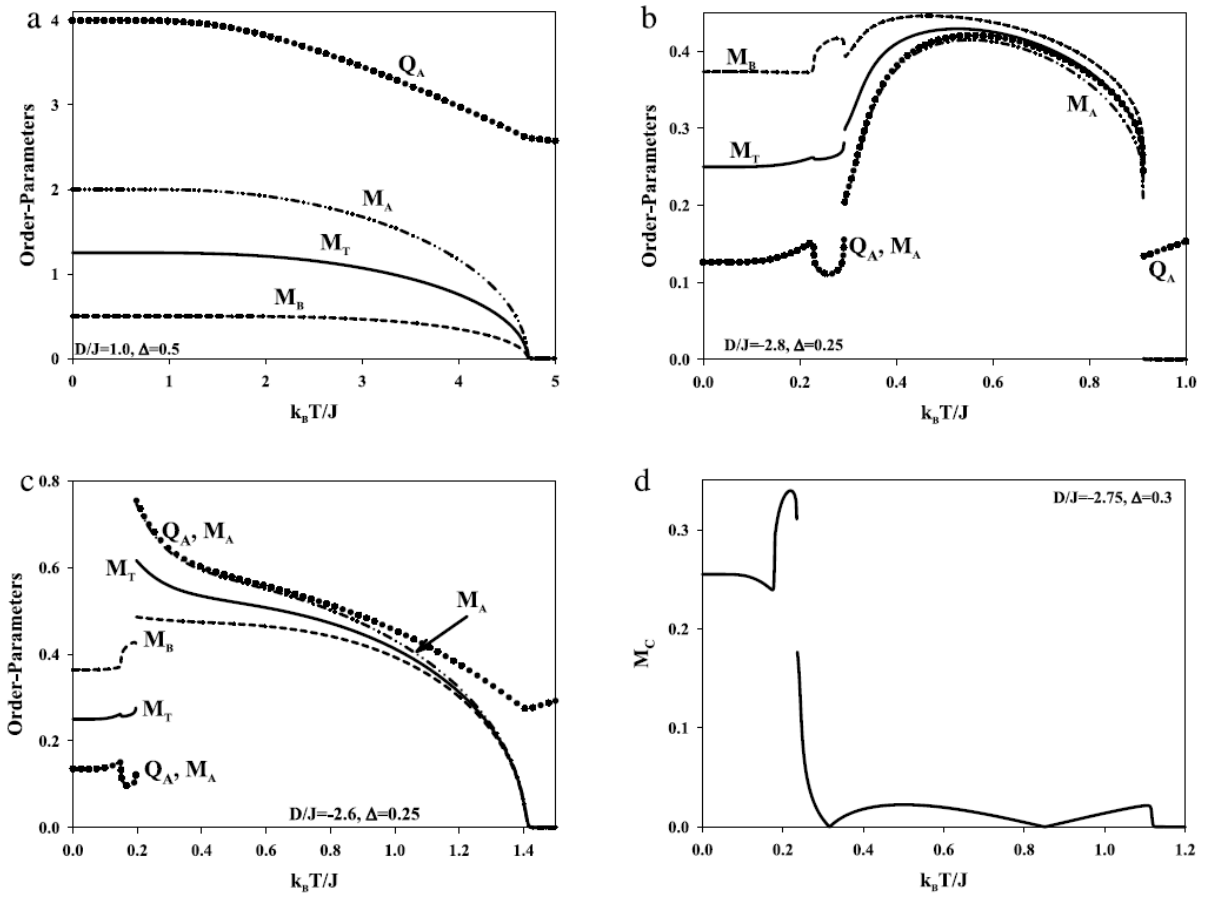
Kare kafes için düzen parametreleri ve serbest enerjinin sıcaklıkla olan değişimleri detaylıca incelendi. Grafiklerde siyah (gri) çizgiler kararlı (kararsız) durumlara ait çözümleri göstermektedir. Şekil 1(a), $D/J = -1.3$ ve $\Delta = 0.0$ elde edilmiş olup ikinci- ve birinci- seviye faz geçiş sıcaklıkları T_C ve T_I vermektedir. Manyetizasyon eğrileri T_C 'de sürekli bir biçimde sıfıra gitmekte, quadrupole moment aynı sıcaklıkta küçük bir çıkıntı yapmakta ve serbest enerji ise süreklilik göstermektedir. T_I sıcaklığında ise bütün düzen parametreleri ve serbest enerji bir atlama yapmaktadır. Görüldüğü gibi M_A ve Q_A sıfır sıcaklıkta 1.0'in biraz üzerinden başlamakta, bilindiği üzere bu parametreler yüksek pozitif kristal alan değerlerinde sırasıyla 2.0 ve 4.0'ten başlamaktadır, M_B ise beklendiği gibi 0.5 değerini almaktadır. Kararsız durumlar ise daha düşük değerlerden başlamakta ve sıcaklık arttıkça artarak T_I sıcaklığında kararlı durum değerlerine atlama yapmaktadırlar. Serbest enerji beklenildiği gibi kararsız çözümler için daha yüksek değerlerde başlar ki bunlar da küçük grafiklerde gösterilmiştir. Buna ilaveten serbest enerjinin bu kararsız çözümleri de T_I 'de kararlı çözüm değerlerine atlamaktadır. Şekil 1(b) ise $D/J = -1.5$ ve $\Delta = 0.0$ değerleri için elde edilmiştir. Görüldüğü gibi sistem ilk önce bir T_I vermekte daha sonra ise alt örgü manyetizasyonları eşit olmakta ki bu telafi sıcaklığını T_{comp} işaret etmekte ve daha sonra ise T_C vermektedir. Şekil 1(c) $D/J = -1.77$ ve $\Delta = 0.25$ değerleri için elde edilmiş olup iki adet T_I sıcaklığı sergilemektedirler. İlk T_I 'de bütün parametreler kararsız değerlerinden kararlı değerlerine atlarken ikinci T_I 'de ise manyetizasyonlar sıfıra atlamakta, quadrupole moment farklı bir değere atlamakta ve serbest enerji ise sürekli olarak devam etmektedir. Son olarak Şekil 1(d) $D/J = -1.95$ ve $\Delta = 0.75$ için hesaplanmış olup üç adet T_I vermektedir. Kararsız çözümler ilk T_I 'de kararlı çözümlere, ikinci T_I 'de farklı sonlu değerlere ve üçüncü T_I 'de ise yine manyetizasyonlar sıfıra, quadrupole

moment ve serbest enerji ise farklı sonlu değerlere atlamaktadır. Görüldüğü üzere farklı sıcaklıklarda iki farklı telafi sıcaklığı elde edilmiştir ki buda faz diyagramlarında görüleceği gibi reentrant davranışının temel sebebidir.



Şekil 1- Düzen parametreleri ve serbest enerjinin $z=4$ için sıcaklığa göre değişimleri: (a) $\Delta = 0.0$, $D/J = -1.3$, (b) $\Delta = 0.0$, $D/J = -1.5$, (c) $\Delta = 0.25$, $D/J = -1.77$ ve (d) $\Delta = 0.75$, $D/J = -1.95$.

Basit kübik kafes için elde edilen düzen parametrelerinin sıcaklığa göre değişimi de kare kafes ile elde edilen sonuçlara benzerdir. Şekil 2(a), $\Delta = 0.5$ ve $D/J = 1.0$ için elde edilmiş olup düzen parametrelerinin davranışını T_c sıcaklığında gösterir. Şekil 2(b) ise düzen parametrelerinin iki kez T_t vermesi durumunda elde edilmiş olup, $\Delta = 0.25$ ve $D/J = -2.8$ değerlerinde hesaplanmıştır. Bir T_t ve bir T_c 'nin sergilendiği Şekil 2(c) ise $\Delta = 0.25$ ve $D/J = -2.6$ için elde edilmiştir. Son olarak Şekil 2(d)'de M_c 'nin termal davranışı $D/J = -2.75$ ve $\Delta = 0.3$ için elde edilmiş olup iki telafi sıcaklığı mevcuttur bu sıcaklıklarda M_c , T_c 'den önce iki kez sıfıra gider. Koordinasyon sayısı z arttıkça verilen aynı Δ ve D/J değerlerinde kritik sıcaklıklar daha yüksek değerlere ulaşmakta ve faz geçişleri daha yüksek negatif kristal alan değerlerinde de gözükmemektedir.

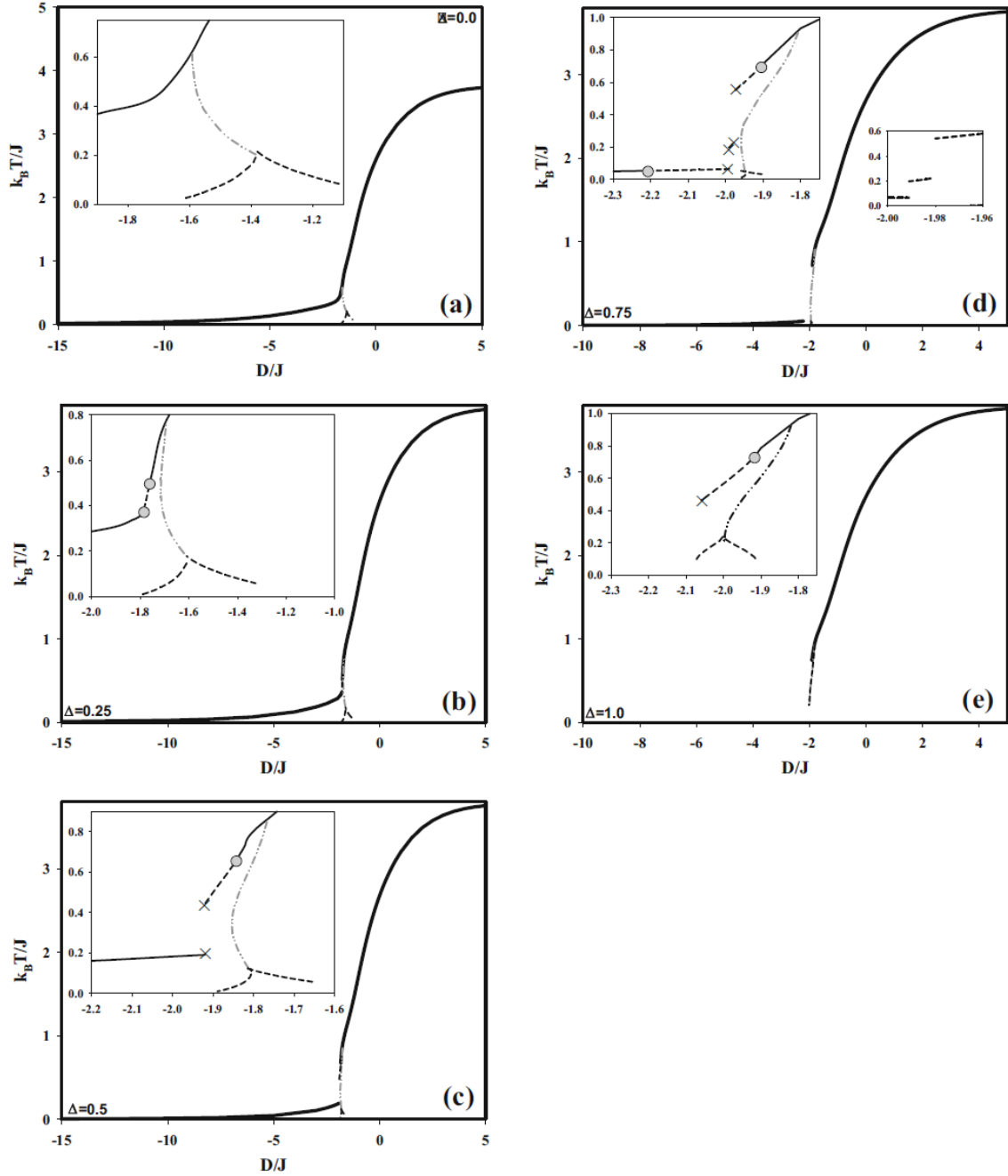


Şekil 2- Düzen parametrelerinin $z=6$ için termal değişimleri: (a) $\Delta = 0.5$ ve $D/J = 1.0$, (b) $\Delta = 0.25$ ve $D/J = -2.8$, (c) $\Delta = 0.25$ ve $D/J = -2.6$, (d) $\Delta = 0.3$ ve $D/J = -2.75$ için iki telafi sıcaklığının elde edildiği M_C 'nin termal değişimi.

Düzen parametreleri ve serbest enerjinin termal değişimleri çalışıldıktan sonra artık faz diyagramlarını vermeye hazırız. Faz diyagramlarında sürekli, kesikli ve kesikli-noktalı çizgiler sırasıyla ikinci- ve birince seviye faz çizgilerine ve telafi sıcaklığı çizgilerine karşılık gelmektedir. Siyah dolgulu üçgenler üçlü kritik ve gri dolu halkalar izole olmuş kritik noktaları ifade etmektedir. En yüksek sıcaklıklardaki T_C yada T_I çizgileri paramanyetik fazları düzenli fazlardan ayırt etmektedir. Δ 'nın farklı değerlerinde modelimiz bazı özel modellere indirgenmektedir öyle ki $\Delta=1.0$ karma-spin Ising modeline, $\Delta=0$ XYZ modeli olarak adlandırılan Heisenberg modeline ve Δ 'nın ara değerlerdeki durumu ise değiş-tokuş anizotropisini dahil eden XYZ modeline karşılık gelmektedir.

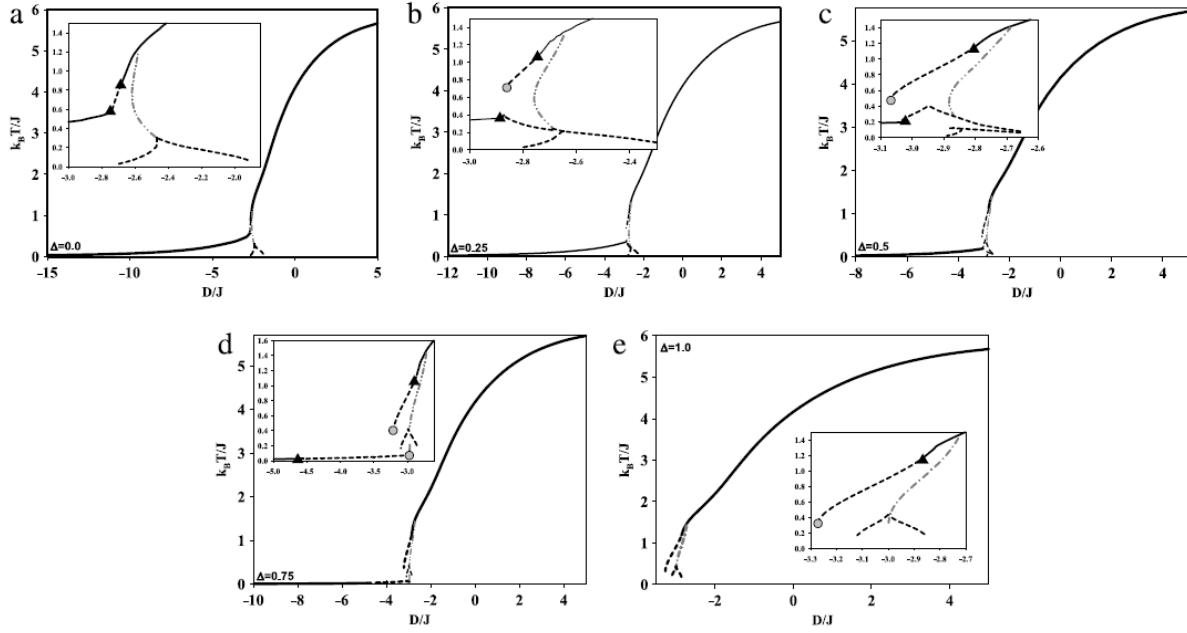
Modelin ilk faz diyagramları (D/J , $k_B T/J$) düzlemlerinde verilen Δ değerlerinde elde edilmiştir. Şekil 3, $z=4$ için yani kare kafes durumunda elde edilmiştir. Şekil 3(a) $\Delta=0.0$ için elde edilmiştir. Görüldüğü gibi T_C çizgisi D/J daha negative oldukça sıcaklığı azalmakta ve

sonunda sıfıra gitmektedir. Bu sonuç $\Delta=1.0$ durumundaki Ising modelinden farklıdır ki orada $z=4$ iken kritik sıcaklıklar $D/J \approx -2.0$ 'de son bulmaktadır oysa burada çok daha yüksek negative D/J değerlerine ulaşılmaktadır. Dolayısı ile Δ 'nın varlığı T_c çizgisinin çok yüksek negative D/J değerlerine kadar kalıcı olmasına sebebiyet verir ki benzer sonuçlar [3]'te verilen Şekil 2 ve 3 ile benzerlik içerisindedir. Kararsız olan birinci-seviye faz çizgilerinin iki kanadı vardır. Telafi sıcaklığı çizgisi T_c -çizgilerinden başlayıp T_t çizgileri üzerinde sona ermektedir. Δ değerleri arttıkça faz çizgileri de çok fazla değişim göstermektedir. Şekil 3(b) $\Delta = 0.25$ için elde edilmiştir. Bu şekilde T_c -çizgisi kısa bir T_t -çizgisi kısmına sahip olup iki üçlü kritik noktada birleşmişlerdir. Δ değeri biraz daha arttırıldığında $\Delta = 0.5$, Gör Şekil 3(c), bir önceki şekildeki alt üçlü kritik nokta yerini izole kritik noktaya bırakmıştır. Aradaki boşluktan sonra ikinci izole kritik noktadan T_c çizgisi başlar ve negative D/J değerlerine doğru devam eder. Telafi sıcaklığı çizgisi reentrant özelliği göstermektedir ki buda iki telafi sıcaklığı noktasının varlığından dolayıdır. Şekil 3(d)'de T_t çizgilerinin üç kısmı vardır ve $\Delta = 0.75$ için elde edilmiştir : İlki T_c çizgisinden başlar ve izole kritik noktada son bulur, bu arada bir çizgi yoktur yani faz geçişi olmayan bir bölge vardır, daha sonra iki izole edilmiş kritik nokta arasında kısa bir T_t -çizgisi mevcuttur, yine bir boşluk ve daha sonra izole edilmiş kritik noktadan başlayıp üçlü kritik noktada son bulan son bir T_t -çizgisi daha vardır. Elde edilen son faz diyagramı karma-spin Ising modelini vermekte olup $\Delta = 1.0$ için hesaplanmıştır (Gör Şekil 3(e)). Bu şekil referanslar [8,9]'de verilen Şekil 4'lerle kalitatif olarak uyumludur, [8]'de aynı zamanda etkin-alan teorisi sonuçları da verilmiştir. Bu çalışma diğer çalışmalarla kıyaslandığında sıcaklıkları daha yüksek değerlere gitmektedir. Etkin-alan teorisi ve Monte-Carlo simülasyonu sonuçları $z=4$ için üçlü kritik nokta verirken [8], Bethe kafesi sonuçları üçlü kritik nokta vermemektedir [9]. Bu şekilde T_t -çizgisi izole edilmiş kritik noktada son bulur ve başka çözümün elde edilemediği bir boşluk vardır. Burada verilen uygun değerlerde bir tek telafi sıcaklığı elde edilmiştir. Sonuç olarak, kritik çizgilerin sıcaklıkları Δ arttıkça artmaktadır. Düşük negative D/J değerlerine doğru uzanan T_c çizgileri Δ arttıkça sağa doğru hareket eder ve $\Delta=1.0$ için artık gözükmez. Kararsız T_t çizgileri Δ arttıkça düşük negative D/J değerlerine doğru kayar. Kararlı T_t -çizgileri sadece $D/J=-2.0$ civarında gözükür ve daima üçlü kritik noktalarla T_c çizgilerine bağlanırlar.



Şekil 3- $(D/J, k_B T/J)$ düzlemlerinde verilmiş Δ değerlerinde faz diyagramları; (a) $\Delta = 0.0$, (b) $\Delta = 0.25$, (c) $\Delta = 0.5$, (d) $\Delta = 0.75$ ve (e) $\Delta = 1.0$. Küçük grafikler detayları belirgin hale getirmek için verilmiştir. Burada gri çemberler ve çarpılar sırasıyla üçlü kritik noktaları ve izole edilmiş kritik noktaları ifade etmektedir.

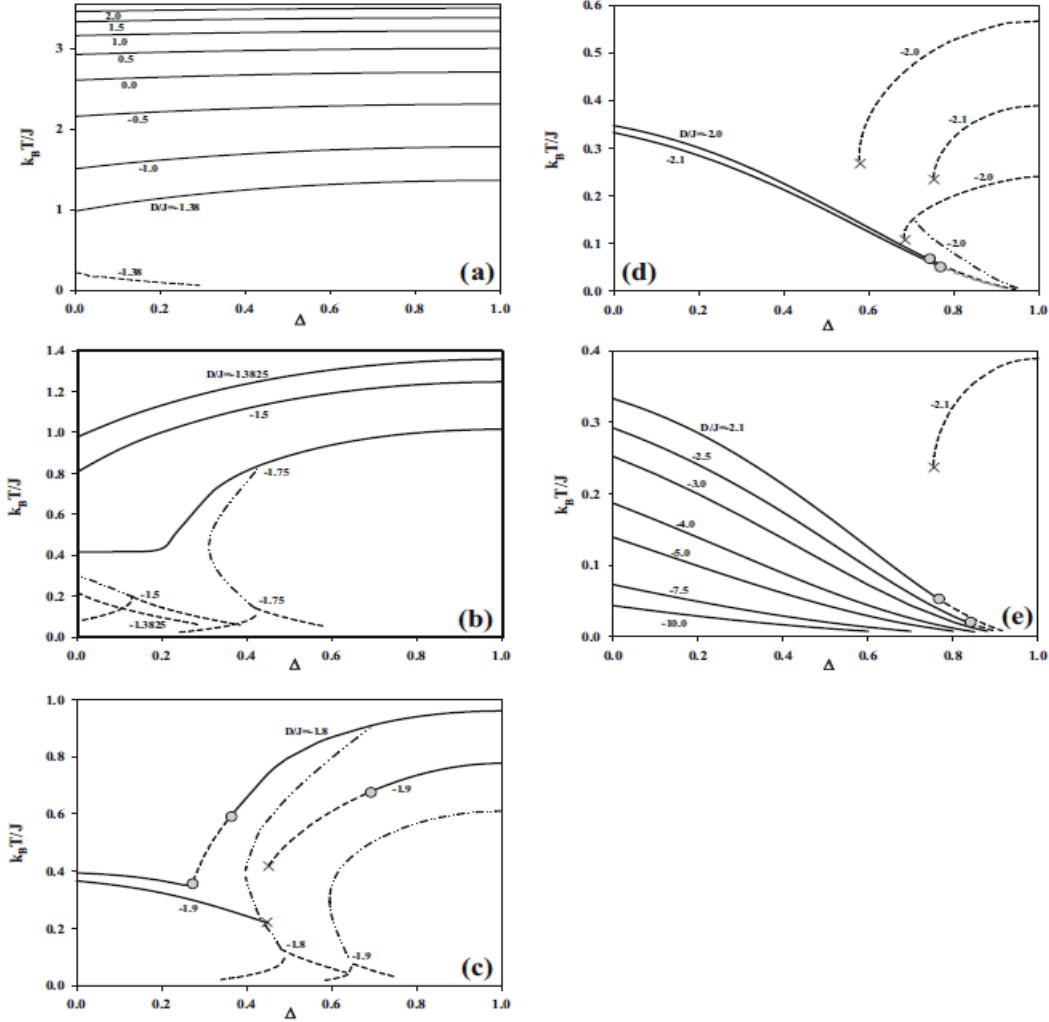
Basit kübik kafes için, $z=6$, için aynı düzlemde elde edilen grafikler, Şekil 4, $z=4$ için olan grafiklerle nitel olarak tamamen benzese de nicel olarak farklılıklar göstermektedir. $z=6$ için elde edilen faz diyagramlarında kritik sıcaklıklar daha yüksek sıcaklıklarda ve daha yüksek D/J değerlerinde gözükmektedir. $z=4$ için Δ 'nın yüksek değerlerinde gözlemlenen kritik olaylar $z=6$ 'nın daha düşük değerlerinde gözlenmektedir.



Şekil 4- $(D/J, k_B T/J)$ düzlemlerinde verilmiş Δ değerlerinde faz diyagramları; (a) $\Delta = 0.0$, (b) $\Delta = 0.25$, (c) $\Delta = 0.5$, (d) $\Delta = 0.75$ ve (e) $\Delta = 1.0$. Küçük grafikler detayları belirgin hale getirmek için verilmiştir. Burada dolu üçgenler ve gri dolgulu halkalar sırasıyla üçlü kritik noktaları ve izole edilmiş kritik noktaları ifade etmektedir.

Bu projenin son faz diyagramları $(\Delta, k_B T/J)$ düzlemlerinde verilen D/J değerleri için hem $z=4$ ve hem de $z=6$ için elde edilmiştir. İlk önce $z=4$ için olan faz diyagramlarını verelim: Şekil 5(a) $D/J = 2.0, 1.5, 1.0, 0.0, -0.5, -1.0$ ve -1.38 değerleri için elde edilmiş olup sadece T_c -çizgileri mevcuttur. Buna ilaveten -1.38 değeri için kararsız T_t -çizgisi de elde edilmiştir. Buradaki kritik çizgilerden görüldüğü üzere kritik çizgilerin sıcaklıkları D/J ya da Δ arttıkça artmaktadır. Şekil 5(b) D/J 'nin $-1.3825, -1.5$, ve -1.75 değerlerinde elde edilmiştir. İlk değer -1.3825 'de elde edilen kritik çizgiler bir önceki şekildeki $D/J = -1.38$ şekli ile benzerdir. İkinci kritik çizgiler iki kanatlı kararsız T_t -çizgilerinin yanı sıra telafi sıcaklığı çizgisi de vermektedir. $D/J = -1.75$ için elde edilen kritik çizgiler kararsız T_t -çizgilerinin daha yüksek Δ değerlerine kaydığını ve telafi çizgisinin reentrant davranışı sergilediğini göstermektedir. Şekil 5(c), $D/J = -1.8$ ve -1.9 için elde edilmiştir. $D/J = -1.8$ olduğunda, $D/J = -1.5$ ve -1.75 için elde edilen kritik çizgilerin yanı sıra iki üçlü kritik nokta arasında gözükten kararlı bir T_t -çizgisi de mevcuttur. $D/J = -1.9$ olduğunda ise T_t -çizgisi üçlü kritik noktadan başlar ve izole edilmiş kritik noktada sona erer. Yine çözümün var olmadığı bir bölge vardır. Sonrasında izole edilmiş kritik noktadan T_c - çizgisi başlar ve sıcaklığı Δ azaldıkça artar. Buna ilaveten, sağa kaymanın yanı sıra, kararsız T_t -çizgileri $D/J = -1.8$ ile

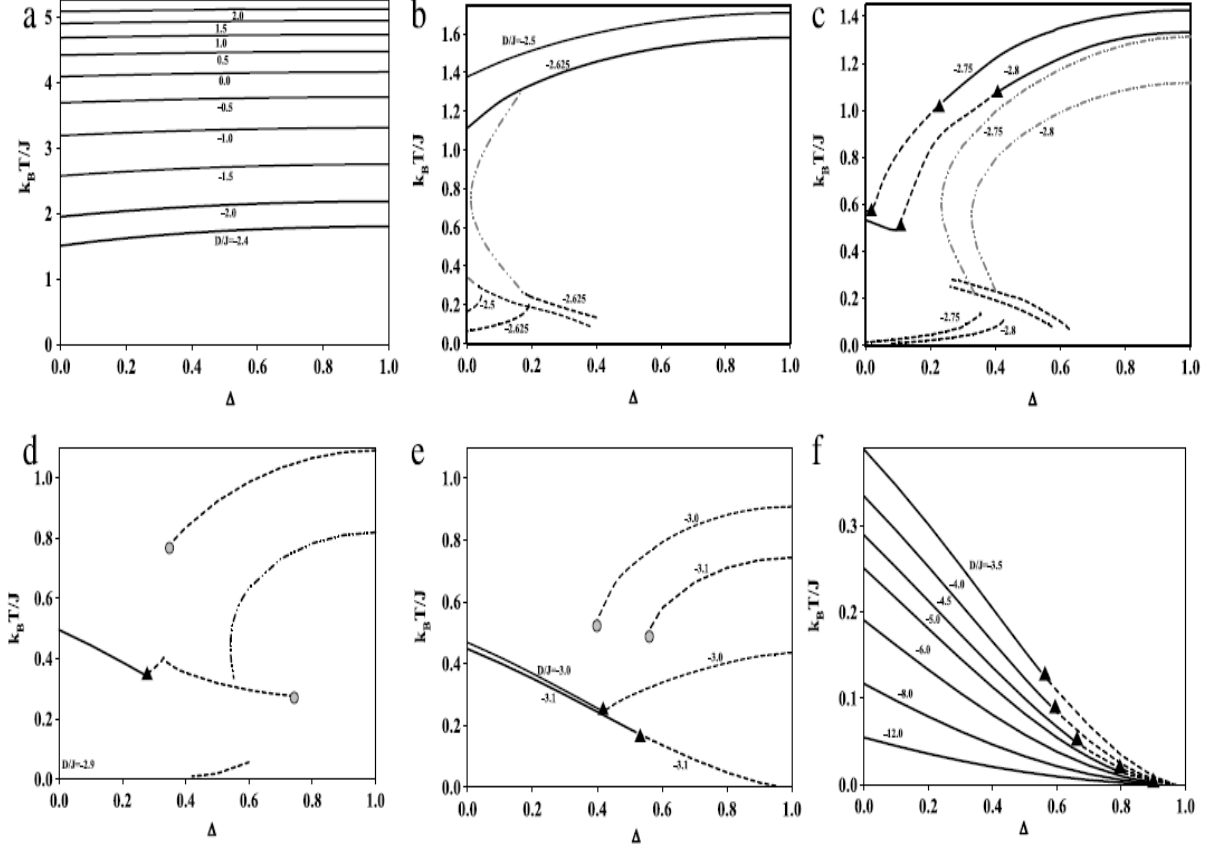
verilenle kıyaslandığında daha küçük bir alan sınırlar. Şekil 5(d) iki kanatlı kararsız T_c -çizgileri artık $D/J = -2.0$ ve -2.1 'de gözükmemektedir. Bunun yerine iki (bir) kararsız T_c -çizgilerini ($\Delta=1.0$ 'de başlar ve Δ azaldıkça sıcaklıkları azalır ve izole edilmiş noktalarda son bulurlar.



Şekil 5- $z=4$ için $(\Delta, k_B T/J)$ düzlemlerinde verilmiş D/J değerlerinde faz diyagramları; (a) 2.0, 1.5, 1.0, 0.5, 0.0, -0.5, -1.0, ve -1.38, (b) -1.3825, -1.5 ve -1.75 (c) -1.8 ve -1.9, (d) -2.0 ve -2.1, ve (e) -2.1, -2.5, -3.0, -4.0, -5.0, -7.5, ve -10.0.

Telafi sıcaklığı da $D/J=-2.1$ için artık yok olmuştur. T_c -çizgileri $\Delta = 0.0$ 'dan başlamakta ve Δ arttıkça sıcaklıkları azalmakta ve üçlü kritik noktada son bulmaktadırlar. Buradan başlayan T_c -çizgileri $\Delta=1$ 'e doğru azalarak gitmekte ve son bulmaktadırlar. Buna ilaveten, D/J daha negative oldukça üçlü kritik noktalar daha yüksek Δ değerlerine doğru kaymaktadırlar. Son faz diyagramı olan Şekil 5(e) T_c -çizgilerinin D/J daha negative oldukça yok olmaya başlar.

Son olarak ta yine aynı düzlemde $z=6$ için olan faz diyagramlarını verelim. Bu durumda yine faz diyagramlarımız $z=4$ ile olanlar ile nitel olarak uyumluluk sergilerken yine nicel olarak farklılıklar göstermektedir. Şekillerden bu nicel farklılıklar aşikardır.



Şekil 6- $z=6$ için $(\Delta, k_B T/J)$ düzlemlerinde verilmiş D/J değerlerinde faz diyagramları; (a) 2.0, 1.5, 1.0, 0.5, 0.0, -0.5, -1.0, -1.5, -2.0 ve -2.4, (b) -2.5 ve -2.625, (c) -2.75 ve -2.8, (d) -2.9, (e) -3.0 ve -3.1 ve (f) -3.5, -4.0, -4.5, -5.0, -6.0, -8.0 ve -12.0.

Sonuç olarak, bu projede, karma spin-2 ve spin-1/2 Hesienberg modelinde değiş-tokuş enerjisi ve kristal alan etkileri Oguchi yaklaşımı kullanılarak kare ve basit kübik kafes üzerinde çalışılmıştır. Düzen parametrelerinin, manyetik dipol ve kuadrupol moment, ve serbest enerjinin sıcaklıkla olan değişimleri incelenerek sistemin mümkün olan düzlemlerdeki faz diyagramları elde edilmiştir. Detaylı faz diyagramları $(D/J, k_B T/J)$ ve $(\Delta, k_B T/J)$ düzlemlerinde sırasıyla verilen Δ ve D/J değerleri için elde edilmiştir. Elde edilen faz diyagramlarında kararlı ya da kararsız olsun bütün çözümler gösterilmiştir. Modelin üçlü kritik ve izole edilmiş kritik noktaların yanı sıra ikinci- ve birinci seviye faz geçişleri verdiği bulunmuştur. Model aynı zamanda verilmiş sistem parametreleri için iki telafi (compensation) sıcaklığı vermiştir ki buda reentrant olayına sebebiyet vermiştir. Modelin düşük sıcaklık bölgesindeki davranışı çok karmaşıktır ki bundan dolayı bu modelin güvenilirliğinin tespiti

daha ileri seviyede incelenmesi gereklidir. Yapılan çalışmalarımız ile hedeflediğimiz bilimsel sonuçlara ulaşmanın yanı sıra Science Citation Index (SCI)'e giren uluslararası dergilerde iki adet yayın [14,15] ve uluslararası bir adet sözlü sunum [16] yapılmıştır ki bu hedef proje başvurusunda belirtilmişti.

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3- Rapor

Mixed Spin-2 and Spin-1/2 Anisotropic Heisenberg Model in the Oguchi Approximation

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Abstract The exchange anisotropy and crystal field effects for the mixed spin-2 and spin-1/2 Heisenberg model are studied on a square lattice by using the Oguchi approximation. Thermal behaviors of the order-parameters, i.e., magnetizations and quadrupole moment, and free energy are investigated to obtain the possible phase diagrams of the model. Not only the stable solutions but also the possible unstable solutions of the model are illustrated on the phase diagrams. Ten topological phase diagrams are presented which is just enough to understand the critical behavior of the model. It is found that the model yields both second- and first-order transitions, in addition to the tricritical and isolated critical points. The existence of compensation temperatures are also searched and it is found that the model gives two compensations for given system parameters.

Keywords Heisenberg model · Oguchi approximation · Exchange anisotropy · Crystal field · Mixed spin

1 Introduction

The mixed-spin systems are interesting since they give some extra properties, such as the existence of compensation temperatures and richer phase diagrams, when

compared to the single spin systems. They are usually studied in the Ising models for which all the spins lie along the same axis, i.e., z -axis. Giving spins the possibility of aligning in three-dimensional space leads to a more complicated system which is quantum mechanical in nature and it is studied in terms of the Heisenberg models. In addition, spins may interact strongly in one direction than the others, thus, one can intend to add an exchange anisotropy term to study its effects on the phase diagrams. It should also be mentioned that the exact solutions are usually unavailable, therefore, it is always necessary to use some kind of approximations such as the one will be used here. In this work, we wish to investigate the mixed spin-2 and spin-1/2 Heisenberg ferrimagnetic system on a square lattice in the Oguchi approximation.

This mixed-spin system has been studied by using a few techniques: The thermal behaviors of the order-parameters and phase diagrams were studied in the Blume-Capel model for the nearest-neighbor interactions on the Bethe lattice by using the exact recursion equations for the coordination numbers $z = 3, 4, 5$ and 6 [1]. The critical behaviour of a mixed ferrimagnetic Ising system was studied on a square lattice in which the two interpenetrating square sublattices have spins $\sigma(\pm 1/2)$ and $S(\pm 2, \pm 1, 0)$. The exact ground state calculations were carried out and Monte Carlo simulations were performed to obtain the finite-temperature phase diagram of the model [2]. The magnetic properties of a ferromagnetic diamond chain were studied by effective-field theory and Monte Carlo simulation based on the Ising model [3]. The compensation and critical behaviors of the Heisenberg ferrimagnetic system on a square lattice were investigated theoretically by the two-time Green's function technique, which takes into account the quantum nature of Heisenberg spins [4].

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We can also list only two experimental works which study systems with spin-2 and spin-1/2 as: A polymer with a large density of cross-links and an alternating connectivity of radical modules with unequal spin quantum numbers (S), macrocyclic $S = 2$, and cross-linking $S = 1/2$ modules, were designed which permits large net S values for either ferromagnetic or antiferromagnetic exchange coupling between the modules [5]. The second one studies the specific heat data on two samples of $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ with relatively low concentrations of paramagnetic centers and show the presence of both spin-2 and spin-1/2 moments [6].

There are also a few works which study the Heisenberg model in the Oguchi approximations for either mixed-spin or single spin systems and interesting results were obtained. The thermodynamic properties of spin-1/2 anisotropic Heisenberg model with Dzyaloshinsky-Moriya interaction were studied using the Oguchi approximation [7]. The thermodynamic properties of spin-1/2 ferromagnetic system were studied on the simple cubic lattice where the effects of the second-nearest-neighbor exchange interactions on the magnetization, internal energy, heat capacity, entropy and free energy were considered [8]. The effects of both exchange anisotropy and single-ion anisotropy were investigated on the phase diagrams of the mixed spin-1 and spin-1/2 [9], including the compensation temperature studies [10] and including the investigation of magnetic susceptibility [11]. The last work of this kind also considers the effects of both exchange anisotropy and single-ion anisotropy on the phase diagrams and magnetization curves of the ferromagnetic mixed spin-3/2 and spin-1/2 model [12]. It should be mentioned that the Mermin-Wagner theorem states that continuous symmetries cannot be spontaneously broken at finite temperature in systems with sufficiently short-range interactions in dimensions $d \leq 2$ [13]. Thus the OA does not give the results in agreement with the Mermin-Wagner theorem for the planar isotropic Heisenberg model, i.e., $q = 4$, since all the mixed-spin 2 and 1/2 systems are studied for $q = 4$ only [1–4], we have preferred to study the $q = 4$ case.

Thus, we consider the effects of exchange anisotropy and crystal field for the mixed spin-2 and spin-1/2 Heisenberg model on a square lattice by using the Oguchi approximation. The detailed phase diagrams are obtained on the $(D/J, k_B T/J)$ and $(\Delta, k_B T/J)$ planes by investigating the thermal variations of the order-parameters and free energy. The phase lines are classified in terms of their stabilities by comparing the free energy values.

The next section is devoted to the formulation of Heisenberg model in the Oguchi approximation. The last section includes the phase diagrams and some of the illustrations for thermal variations of the order-parameters and free energy. It also includes discussions, conclusion, and comparisons.

2 Formulation

The Hamiltonian for the mixed spin- S_A and spin- S_B can be given as

$$\hat{\mathcal{H}} = -J \sum_{\langle ij \rangle} [(1 - \Delta)(\hat{S}_{iA}^x \hat{S}_{jB}^x + \hat{S}_{iA}^y \hat{S}_{jB}^y) + \hat{S}_{iA}^z \hat{S}_{jB}^z] - D \sum_{i \in A} (\hat{S}_{iA}^z)^2, \quad (1)$$

where $\hat{S}_{iA}^\delta$ and $\hat{S}_{jB}^\delta$ with $(\delta = x, y, z)$ are the components of spin-2 and spin-1/2 operators for the sublattices A and B, respectively. J is the nearest-neighbor (NN) bilinear exchange interaction parameter, D is the crystal field acting only to the sites with spin-2, i.e., only on sublattice A, and Δ is the exchange anisotropy parameter with $0 \leq \Delta \leq 1$.

In the Oguchi approximation, the NN pair interactions between the spin components are treated exactly and the rest of interactions are replaced with the effective field terms as it is usually done in the mean-field approximations. Therefore, the effective Oguchi Hamiltonian for a pair of spins is given by

$$\hat{\mathcal{H}}_{ij} = -J[(1 - \Delta)(\hat{S}_{iA}^x \hat{S}_{jB}^x + \hat{S}_{iA}^y \hat{S}_{jB}^y) + \hat{S}_{iA}^z \hat{S}_{jB}^z] - D(\hat{S}_{iA}^z)^2 - h_i \hat{S}_{iA}^z - h_j \hat{S}_{jB}^z \quad (2)$$

where the mean-field terms are given as

$$h_i = (z - 1)JM_B \\ h_j = (z - 1)JM_A \quad (3)$$

with $M_A = \langle \hat{S}_{iA}^z \rangle$ and $M_B = \langle \hat{S}_{jB}^z \rangle$ are the magnetizations of the sublattices, z is the number of NN's and $\langle \dots \rangle$ corresponds to thermal averages.

In order to obtain the formulations of necessary thermodynamic functions in the Heisenberg model, one has to solve the eigenvalue equation

$$\hat{\mathcal{H}}_{ij} |n\rangle = E_n |n\rangle, \quad n = 1, 2, \dots, 10 \quad (4)$$

where $|n\rangle$ are the eigenvectors and E_n are the eigenvalues. Thus, one have to consider the direct products of the possible vectors $|s_A, m_{s_A}\rangle_i$ for spin-2 and $|s_B, m_{s_B}\rangle_j$ for spin-1/2. As a result of the direct product, i.e., $|s_A, m_{s_A}\rangle_i \otimes |s_B, m_{s_B}\rangle_j$, one gets ten possible base vectors that are given as

$$\begin{aligned} |I\rangle &= |2, 2\rangle_i |1/2, 1/2\rangle_j, & |II\rangle &= |2, 2\rangle_i |1/2, -1/2\rangle_j, \\ |III\rangle &= |2, 1\rangle_i |1/2, 1/2\rangle_j, & |IV\rangle &= |2, 1\rangle_i |1/2, -1/2\rangle_j, \\ |V\rangle &= |2, 0\rangle_i |1/2, 1/2\rangle_j, & |VI\rangle &= |2, 0\rangle_i |1/2, -1/2\rangle_j, \\ |VII\rangle &= |2, -1\rangle_i |1/2, 1/2\rangle_j, & |VIII\rangle &= |2, -1\rangle_i |1/2, -1/2\rangle_j, \\ |IX\rangle &= |2, -2\rangle_i |1/2, 1/2\rangle_j, & |X\rangle &= |2, -2\rangle_i |1/2, -1/2\rangle_j \end{aligned} \quad (5)$$

which are used to obtain the matrix representation of the eigenvalue equation and where $\otimes$ is omitted for simplicity. Thus, in this representation, one obtains a 10×10 matrix

whose elements are calculated from $E_{ij} = \langle i | \hat{\mathcal{H}}_{ij} | j \rangle$ with $i, j = I, II, \dots, X$. The non-zero elements are found as

$$\begin{aligned} E_{11} &= -J - 4D - 2h_i - h_j/2, & E_{22} &= J - 4D - 2h_i + h_j/2, \\ E_{33} &= -J/2 - D - h_i - h_j/2, & E_{44} &= J/2 - D - h_i + h_j/2, \\ E_{55} &= -h_j/2, & E_{66} &= h_j/2, \\ E_{77} &= J/2 - D + h_i - h_j/2, & E_{88} &= -J/2 - D + h_i + h_j/2, \\ E_{99} &= J - 4D + 2h_i - h_j/2, & E_{1010} &= -J - 4D + 2h_i + h_j/2, \\ E_{23} &= E_{32} = -J(1 - \Delta), & E_{45} &= E_{54} = -\sqrt{6}J(1 - \Delta)/2, \\ E_{67} &= E_{76} = -\sqrt{6}J(1 - \Delta)/2, & E_{89} &= E_{98} = -J(1 - \Delta). \end{aligned} \quad (6)$$

Thus, it is clear from the above matrix elements that the matrix representation of $\hat{\mathcal{H}}_{ij}$ in this base is symmetric. As a last step, we need to find the eigenvalues and eigenvectors, i.e., correct superposition of the base vectors, of this matrix. Actually, the latter is not intended to be given in here, since we only need the eigenvalues to get our thermodynamic functions. The calculated eigenvalues are found as

$$\begin{aligned} E_{1,2} &= -4D \pm 2h_i \pm h_j/2 - J, \\ E_{3,4} &= \left[-10D + 6h_i + J \pm \left[36D^2 - 24Dh_i + 4h_i^2 + 24Dh_j - 8h_i h_j \right. \right. \\ &\quad \left. \left. + 4h_j^2 - 36DJ + 12h_i J - 12h_j J + 9J^2 + 64J^2 \right]^{1/2} \right] / 4, \\ E_{5,6} &= \left[-10D - 6h_i + J \pm \left[36D^2 + 24Dh_i + 4h_i^2 - 24Dh_j - 8h_i h_j \right. \right. \\ &\quad \left. \left. + 4h_j^2 - 36DJ - 12h_i J + 12h_j J + 9J^2 + 64J^2 \right]^{1/2} \right] / 4, \\ E_{7,8} &= \left[-4D - 4h_i + 2J \pm \left[(4D + 4h_i - 2J)^2 - 16(2Dh_j + 2h_i h_j - h_j^2 \right. \right. \\ &\quad \left. \left. - h_j J - 24J^2) \right]^{1/2} \right] / 8, \\ E_{9,10} &= \left[-4D + 4h_i + 2J \pm \left[(4D - 4h_i - 2J)^2 - 16(-2Dh_j + 2h_i h_j - h_j^2 \right. \right. \\ &\quad \left. \left. + h_j J - 24J^2) \right]^{1/2} \right] / 8 \end{aligned} \quad (7)$$

with $J' = \frac{J}{2}(1 - \Delta)$. They are used in the below equation to calculate the partition function

$$Z = \text{Tr}_{ij} [\exp(-\beta \hat{\mathcal{H}}_{ij})] = \sum_{i=1}^n e^{-\beta E_i} \quad (8)$$

with $\beta = 1/k_B T$ and k_B is the Boltzmann constant. In many statistical physics problems, the calculation of Z has the main importance since all needed thermodynamic functions can be obtained from it.

Thus, the magnetization and quadrupole moment for the sublattice A with spin-2 can be calculated respectively from

$$M_A = \frac{1}{\beta Z} \frac{\partial Z}{\partial h_i} \quad (9)$$

and

$$Q_A = \frac{1}{\beta Z} \frac{\partial Z}{\partial D}. \quad (10)$$

Similarly, the magnetization for the sublattice B is calculated from

$$M_B = \frac{1}{\beta Z} \frac{\partial Z}{\partial h_j}. \quad (11)$$

Finally, the free energy of the model can be obtained by using

$$F = -(1/\beta) \ln Z + J(z - 1)M_A M_B. \quad (12)$$

The compensation temperatures T_{comp} , which is caused by different responses of the sublattice magnetizations to temperature changes, can be calculated by obtaining the crossing points between the absolute values of the sublattice magnetizations;

$$|M_A(T_{comp})| = |M_B(T_{comp})| \quad (13)$$

or when the net magnetization goes to zero, i.e.,

$$M_{NET} = |M_A(T_{comp})| - |M_B(T_{comp})| = 0.0 \quad (14)$$

with the conditions

$$\text{sign}[M_A(T_{comp})] = -\text{sign}[M_B(T_{comp})], \quad T_{comp} < T_c. \quad (15)$$

Thus, these conditions warrant that the two sublattice magnetizations cancel each other at the compensation temperatures.

These are all the main ingredients to obtain the phase diagrams of the model. For this purpose, one has to study the thermal variations of the order-parameters by using an iteration procedure. Thus, the numerical calculations may lead to different solutions for different initial values of the order-parameters. The free energy is used to classify these solutions with respect to their stabilities. The next section is devoted for this.

3 The Results and Conclusions

Before going into the illustrations, we should note that $\Delta = 1.0$ corresponds to mixed-spin Ising model, $\Delta = 0.0$ corresponds to the Heisenberg model called as XYZ model, for the intermediate values of Δ it is still XYZ model with the effects of exchange anisotropy term.

As a result of numerical calculations, the phase diagrams of the model are obtained on the $(D/J, k_B T/J)$ and $(\Delta, k_B T/J)$ planes for given values of Δ and D/J , respectively, by investigating the thermal variations of the order-parameters and free energy. In the phase diagrams, the solid, dashed, and dashed-dotted lines correspond to the second- and first-order phase transition temperatures and

compensation temperatures, respectively. The gray-filled circles correspond to tricritical points while the times are used to indicate the isolated critical points of the critical lines. It should also be mentioned that the T_c -lines and T_t -lines connecting at the tricritical points separate the paramagnetic phase regions (above the lines) from the ordered phase regions (below the lines) in the mixed spin Ising models for $z = 4$. The ordered phase regions has two parts: one

extends to higher negative values of D , i.e. $D < -2.0$, and the part with $D > -2.0$ as explained in [9], but we are not going to distinguish them in here.

The first phase diagrams are obtained on the $(D/J, k_B T/J)$ planes for given values of Δ and are illustrated in Fig. 1. Figure 1a is obtained when $\Delta = 0.0$, the solid line, i.e. T_c -line, decrease in temperature as D/J gets more negative and eventually disappears at higher

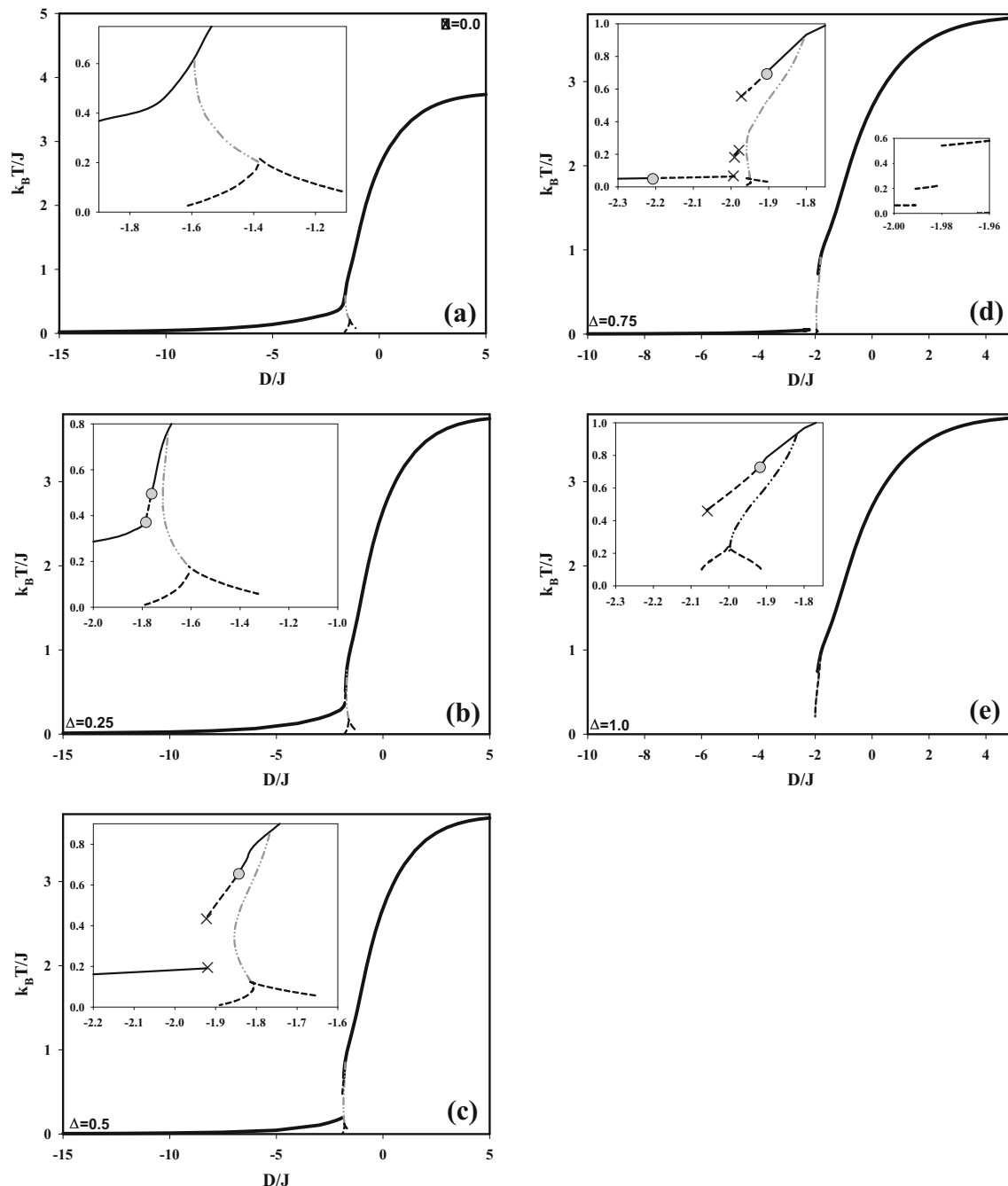


Fig. 1 The phase diagrams on the $(D/J, k_B T/J)$ planes for given values of Δ ; **a** 0.0, **b** 0.25, **c** 0.5, **d** 0.75, and **e** 1.0. The insets are intended to give all the details of the phase lines where the gray circles and times indicate the tricritical and isolated critical points, respectively

negative D/J 's. This result is different than the results when $\Delta = 1.0$, i.e. Ising model results, where the critical line terminates at $D/J \cong -2.0$ for $z = 4$. So, the existence of Δ causes the T_c -lines to be more persistent even at lower negative D/J 's, see also Figs. 2 and 3 of [9]. The unstable portions of the first-order phase lines, i.e., the T_l -lines, has two wings. The compensation temperature line, T_{comp} -line, emerges from the T_c -line and terminates on the T_l -line. As the strength of exchange anisotropy term decreases, the phase diagrams change drastically. Figure 1b is calculated when $\Delta = 0.25$ which is qualitatively similar with Fig. 1a, but now the T_c -line has a small T_l -line portion which is

combined with the T_c -lines at two tricritical points. When Δ is increased further, Fig. 1c for $\Delta = 0.5$, the lower tricritical point of Fig. 1b is now broken from the T_l -line at the isolated critical point. Then, the critical line starts from the second isolated critical point on the T_c -line. In between these two points, no solution is obtained. This may be caused by Δ which drives spin-2 suddenly jump to $1/2$ value which is interesting since spin-2 can have only $\pm 2, \pm 1, 0$. The T_{comp} -line shows reentrant behavior, which is caused by the existence of two compensation temperatures for given system parameters. Figure 1d shows that the T_l -line has three portions: First one starts from the T_c -line

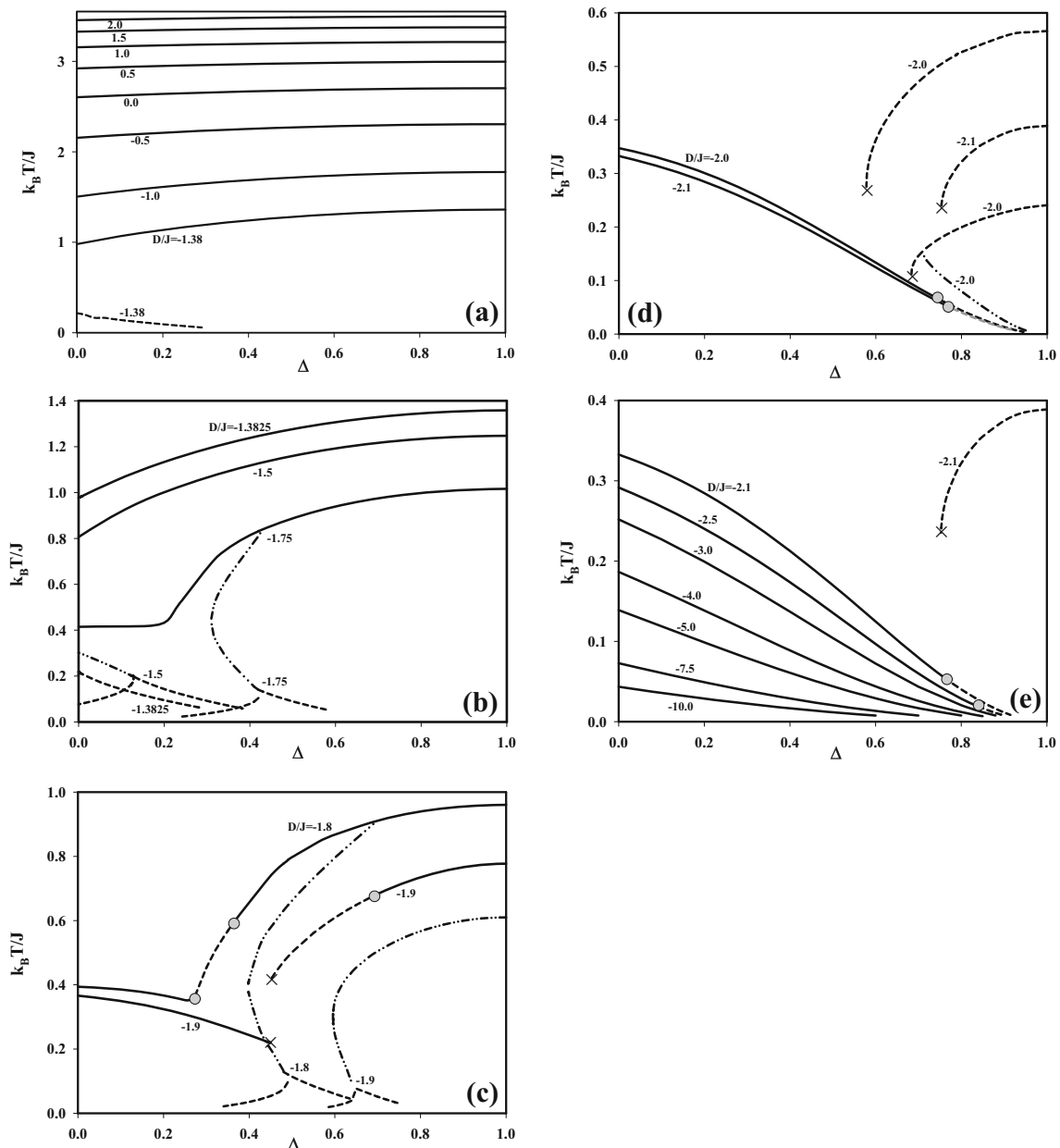


Fig. 2 The phase diagrams on the $(\Delta, k_B T/J)$ planes for given values of D/J ; **a** 2.0, 1.5, 1.0, 0.5, 0.0, -0.5, -1.0, and -1.38, **b** -1.3825, -1.5, and -1.75 **c** -1.8 and -1.9, **d** -2.0 and -2.1, and **e** -2.1, -2.5, -3.0, -4.0, -5.0, -7.5, and -10.0

and terminates at isolated critical point, then there is a space of no solution, then the second T_i -line is seen between two isolated critical points, then there is a space again, and then the third T_i -line appears starting from isolated critical point and ending at tricritical point. The last figure, Fig. 1e, is obtained for $\Delta = 1.0$ corresponding to the mixed-spin Ising model. This figure is similar qualitatively with Fig. 4 of [1, 2], the latter also gives the phase line obtained by the effective field theory (EFT). It is clear that the present work over estimates the temperatures when compared with all three results. The EFT does predict a tricritical point as in this work but the Monte Carlo simulation [2] and Bethe lattice results [1] does not predict any tricritical points when $z = 4$. The T_i -line was terminated at the isolated critical point and no other solutions were found. The model yields one compensation at a time. As a conclusion, the temperatures of the critical lines are increased as Δ increased. The T_c -line extending to lower negative D/J values move towards right as Δ increased and disappear for $\Delta = 1.0$. The unstable T_i -lines move to the lower negative D/J 's as Δ is increased. The stable T_i -lines are only seen about $D/J = -2.0$ and always connected to the T_c -lines via tricritical points.

The next phase diagrams are obtained on the $(\Delta, k_B T/J)$ planes for given values of D/J and are given in Figs. 2.

Figure 2a shows only T_c -lines obtained for $D/J = 2.0, 1.5, 1.0, 0.0, -0.5, -1.0$, and -1.38 except for the latter for which the unstable portion of the T_i -line is also seen. It is clear that the temperatures of the critical lines increase gradually as D/J or Δ is increased. Next figures, Fig. 2b, are obtained when $D/J = -1.3825, -1.5$, and -1.75 . The first one is similar with the $D/J = -1.38$ of the previous figure. The second one shows the unstable portions of the T_i -lines with two wings in addition to the T_{comp} -line. The last one shows that the unstable T_i -lines move towards higher Δ 's and T_{comp} -line exhibits reentrant behavior. Figure 2c is obtained for $D/J = -1.8$ and -1.9 . When $D/J = -1.8$, a stable T_i -line is seen in between the two tricritical points in addition to the other lines of $D/J = -1.5$ and -1.75 . For $D/J = -1.9$, the T_i -line starts from the tricritical point and then terminates at isolated critical point. Again there is a space of no solution. Then, the T_c -line starts from the isolated critical point which increase in temperature as Δ is decreased towards zero. In addition to moving right, the unstable T_i -lines cover smaller area when compared with $D/J = -1.8$. The next figure, Fig. 2d, shows the two winged unstable T_i -lines disappear for $D/J = -2.0$ and -2.1 . Instead, we see two (one) unstable T_i -lines for $D/J = -2.0$ (-2.1) starting at $\Delta = 1.0$ and decrease in temperature as Δ increased and

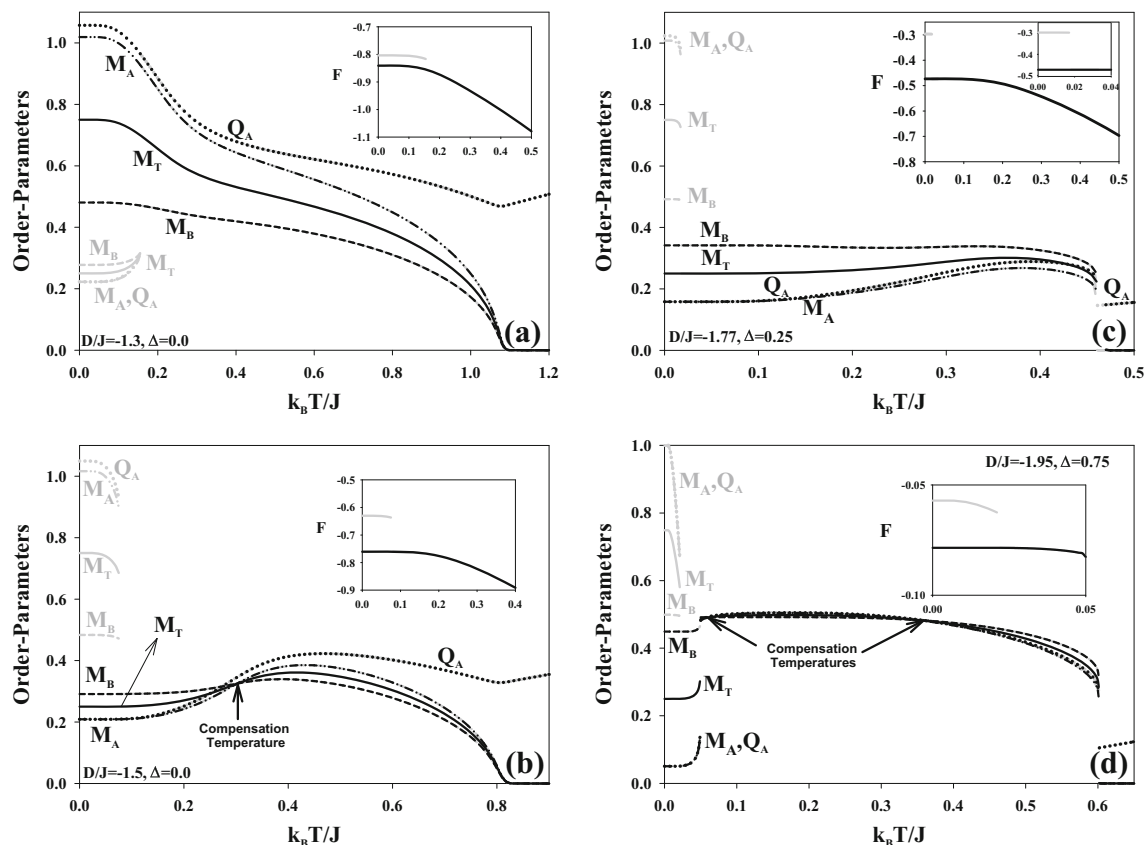


Fig. 3 The thermal variations of the order-parameters and free energy; **a** $\Delta = 0.0$, $D/J = -1.3$. **b** $\Delta = 0.0$, $D/J = -1.5$. **c** $\Delta = 0.25$, $D/J = -1.77$, and **d** $\Delta = 0.75$, $D/J = -1.95$

they terminate at the isolated critical points. The T_{comp} -line is not seen anymore for $D/J = -2.1$. The T_c -lines start at $\Delta = 0.0$ and decrease in temperature as Δ is increased, then terminates at tricritical points from where the T_t -lines emerge which then disappear towards $\Delta = 1.0$. In addition, the tricritical points move to higher Δ 's as D/J becomes more negative. The last figure, Fig. 2e, shows that the T_c -lines start disappearing as D/J becomes more and more negative.

The last figures of this work show the thermal variations of magnetizations and free energy. The latter is especially important to distinguish whether the solutions are stable or not. The black (gray) lines indicate the stable (unstable) solutions. Figure 3a is calculated for $D/J = -1.3$ and $\Delta = 0.0$ at which the magnetizations and free energy must give a T_t at lower and a T_c at higher temperatures (see Fig. 1a). As seen M_A and Q_A start a little above 1.0, which start at 2.0 and 4.0 for higher positive D/J 's, and M_B starts at 0.5 as expected. Thus, it is clear that as D/J becomes more negative the ground state values of M_A and Q_A are lowered. Magnetization lines are continuous and as the temperature increases they decrease in temperature and all go to zero at the T_c where Q_A presents a little kink. The unstable parts start from lower temperatures and gradually increase as temperature increases then they jump to their stable values. Thus, this jump actually occurs at the T_t . The free energy starts from higher values for the unstable solutions as expected which is shown in the inset. In addition, it presents a jump to its stable value at the T_t . The stable part is always continuous. The next figure, Fig. 3b, is obtained when $D/J = -1.5$ and $\Delta = 0.0$. Now, one expects a T_t , a T_{comp} and T_c according to Fig. 1a. This is indeed the case. The unstable solutions start from higher values in comparison to the stable solutions. The sublattice magnetizations M_A and M_B becomes equal at the T_{comp} . Figure 3c is obtained for $D/J = -1.77$ and $\Delta = 0.25$ for which one expects two T_t 's. Again the unstable ones jump to their stable values at the T_t . In addition, the stable magnetization lines jump to zero and Q_A jump to a nonzero value at the second T_t . At the first T_t , F jumps to its stable value while it is continuous at the second T_t . Thus, it is clear that the continuity of F may be indicating also the stability of the solutions. The last figure of this work, Fig. 3d, presents three T_t 's according to Fig. 1d and obtained for $D/J = -1.95$ and $\Delta = 0.75$. The unstable solutions make jumps at a lower temperature which then jump to their stable values. Then, another jump is seen to higher values. Lastly, the third jump is seen to zero values for magnetizations and to a nonzero

value for Q_A . As seen from the inset, F is discontinuous at the first T_t , but it is continuous at the second and last T_t 's. The reason of reentrant behavior is also clear from this figure, i.e., the model presents two T_{comp} 's for given D/J and Δ .

In conclusion, we have studied the exchange anisotropy and crystal field effects for the mixed spin-2 and spin-1/2 Heisenberg model on a square lattice by using the Oguchi approximation. The phase diagrams are calculated by studying the thermal changes of the order-parameters and free energy. In addition to the stable solutions, the unstable solutions of the model are also examined. The model yields both second- and first-order transitions, in addition to the tricritical and isolated critical points. The compensation temperature lines present reentrant behavior so this means that the model gives two compensations for given parameters. Some important conclusions are given during the explanations of figures and whenever possible a few comparisons are also made and similarities are observed. As an important conclusion, even if this mixed-spin system including anisotropy is not studied with any other techniques so far, we see for the case with $\Delta = 1.0$, i.e. [1–4], some shortcomings or maybe some kinds of artifacts at low temperature regions.

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Anisotropic Heisenberg model for the mixed spin-2 and spin-1/2 in the Oguchi approximation on the simple cubic lattice

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HIGHLIGHTS

- The mixed spin-2 and spin-1/2 Heisenberg model is studied on a simple cubic lattice.
- Oguchi approximation to examine the effects of exchange anisotropy and crystal field.
- The phase diagrams are obtained on various planes for given values of Δ and D/J .
- The model yields second and first-order phase transitions.
- The model also gives two compensation temperatures, they exhibit reentrant behavior.

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ABSTRACT

The mixed spin-2 and spin-1/2 Heisenberg model is studied on a simple cubic lattice by using the Oguchi approximation to examine the effects of exchange anisotropy and crystal field. The thermal variations of the order-parameters, i.e. magnetization and quadrupole moment, are investigated to obtain the possible phase diagrams of the model. The detailed phase diagrams are obtained on the $(D/J, k_B T/J)$ and $(\Delta, k_B T/J)$ planes for given values of Δ and D/J , respectively. In the phase diagrams all possible solutions are illustrated whether stable or not. The model yields second and first-order phase transitions, in addition to the tricritical and isolated critical points. The model also gives two compensation temperatures for given system parameters, therefore, they exhibit reentrant behavior. The low temperature behavior of the model is very complicated, therefore, the reliability of the Oguchi approximation should be investigated further.

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1. Introduction

After the detailed investigations of single spin type Ising models, the next logical step was to mixed them up with different spins in various structures. The studies of mixed-spin systems revealed an important property called as the compensation temperature which has many technological applications such as magnetic recording etc. In addition to this, the phase diagrams become much richer, therefore, they also got a lot of attention. In the Ising model the spins can only align along one axis which is usually chosen as the z -axis. When this limitation is lifted, i.e. giving spins the possibility of aligning in three-dimensional space may lead to much more complicated systems which are quantum mechanical in nature and they are studied in terms of the Heisenberg models. In this model, the spin operators do not commute with each other, therefore, there are certain types of uncertainties in the measurement of physical observables. Thus the exact solutions are

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usually unavailable, therefore, it is always necessary to use some kind of approximations which may give some qualitative pictures but usually has many shortcomings. In this work, we wish to investigate the mixed spin-2 and spin-1/2 Heisenberg ferrimagnetic system on a simple cubic lattice in the Oguchi approximation (OA).

The Heisenberg model in the OA was considered for either single-spin or mixed-spin systems and interesting results were obtained. The thermodynamic properties of spin-1/2 anisotropic Heisenberg model with Dzyaloshinskii–Moriya interaction were studied [1]. The same spin system was also considered where the effects of the second-nearest-neighbor exchange interactions on the magnetization, internal energy, heat capacity, entropy and free energy were considered [2]. The effects of both exchange and single-ion anisotropies were investigated on the phase diagrams of the mixed spin-1 and spin-1/2 [3], including the compensation temperature studies [4] and including the investigation of magnetic susceptibility [5]. The similar properties was also considered in the ferromagnetic mixed spin-3/2 and spin-1/2 model [6]. In all these works only the simple cubic lattice structures were considered since Mermin–Wagner theorem states that continuous symmetries cannot be spontaneously broken at finite temperature in systems with sufficiently short-range interactions in dimensions $d \leq 2$ [7]. Thus the OA does not give the results in agreement with the Mermin–Wagner theorem for the planar isotropic Heisenberg model, therefore, in this work we take $z = 6$, i.e. the number of nearest-neighbor spins, corresponding the simple cubic lattice in order not to violate the Mermin–Wagner theorem.

As far as in our knowledge, the mixed spin-2 and spin-1/2 system was mostly considered in the Ising models: The critical behaviors of some mixed ferrimagnetic systems were studied on a square lattice in which the two interpenetrating square sublattices had spins $\sigma(\pm 1/2)$ and $S(\pm 2, \pm 1, 0)$ and the exact ground state calculations were carried out and Monte Carlo (MC) simulations were performed to obtain the finite-temperature phase diagram of the model [8]. The thermal behaviors of the order-parameters and phase diagrams were studied in the Blume–Capel model for the nearest-neighbor interactions on the Bethe lattice by using the exact recursion equations for the coordination numbers $z = 3, 4, 5$ and 6 [9]. The magnetic properties of a ferromagnetic diamond chain were studied by effective-field theory (EFT) and MC simulation based on the Ising model [10]. The only work in terms of Heisenberg model investigated the compensation and critical behaviors on a square lattice theoretically by the two-time Green's function technique, which takes into account the quantum nature of Heisenberg spins [11]. It should be mentioned that in these works usually the effects of crystal field were considered, but for the three-dimensional case the spins may interact strongly in one direction than the others, thus, one can intend to add an exchange anisotropy term to study its effects on the phase diagrams too.

There are not many experimental works including mixed spin-2 and 1/2 system but we can at least give two experimental works such as: A polymer with a large density of cross-links and an alternating connectivity of radical modules with unequal spin quantum numbers (S), macrocyclic $S = 2$, and cross-linking $S = 1/2$ modules, were designed which permits large net S values for either ferromagnetic or antiferromagnetic exchange coupling between the modules [12]. The second one studies the specific heat data on two samples of $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ with relatively low concentrations of paramagnetic centers and show the presence of both spin-2 and spin-1/2 moments [13].

In this work, the effects of exchange anisotropy and crystal field for the mixed spin-2 and spin-1/2 Heisenberg model on a simple cubic lattice are investigated by using the Oguchi approximation. The detailed phase diagrams are obtained on the $(D/J, k_B T/J)$ and $(\Delta, k_B T/J)$ planes for given values of Δ and D/J respectively by investigating the thermal variations of the order-parameters. It is found that the model gives second- and first-order phase transitions and some critical points in addition to compensation temperatures.

The rest of the work is set up as follows: The next section is dedicated to the formulation of Heisenberg model in the Oguchi approximation for the mixed spin-2 and 1/2 system. The third section comprises from the phase diagrams and some of the illustrations for thermal variations of the order-parameters in addition to some comparisons whenever possible. The last section is devoted to brief summary and conclusions.

2. Formulation

The usual Hamiltonian for the mixed spin- S_A and spin- S_B including exchange anisotropy parameter Δ may be given as

$$\hat{H} = -J \sum_{\langle ij \rangle} [(1 - \Delta)(\hat{S}_{iA}^x \hat{S}_{jB}^x + \hat{S}_{iA}^y \hat{S}_{jB}^y) + \hat{S}_{iA}^z \hat{S}_{jB}^z] - D \sum_{i \in A} (\hat{S}_{iA}^z)^2, \quad (1)$$

where S_{iA}^δ and S_{jB}^δ with $(\delta = x, y, z)$ are the components of spin-2 and spin-1/2 operators for the sublattices A and B , respectively. D is the crystal field acting only to the spin-2 sites, i.e. only on sublattice A , J is the nearest-neighbor (NN) bilinear exchange interaction parameter and the exchange anisotropy parameter only lies in the $0 \leq \Delta \leq 1$ range.

In the OA, the NN pair interactions between the spin components are treated exactly and the rest of interactions are replaced with the effective field terms as it is usually done in the mean-field approximations. Therefore, the effective Oguchi Hamiltonian for a pair of spins is given by

$$\hat{H}_{ij} = -J[(1 - \Delta)(\hat{S}_{iA}^x \hat{S}_{jB}^x + \hat{S}_{iA}^y \hat{S}_{jB}^y) + \hat{S}_{iA}^z \hat{S}_{jB}^z] - D(\hat{S}_{iA}^z)^2 - h_i \hat{S}_{iA}^z - h_j \hat{S}_{jB}^z \quad (2)$$

where the mean-field terms are given as

$$\begin{aligned} h_i &= (z - 1)JM_B \\ h_j &= (z - 1)JM_A \end{aligned} \quad (3)$$

with $M_A = \langle \hat{S}_{iA}^z \rangle$ and $M_B = \langle \hat{S}_{jB}^z \rangle$ are the magnetizations of the sublattices, z is the number of NN's and $\langle \dots \rangle$ corresponds to thermal averages.

As in many quantum mechanics problems one has to solve the eigenvalue equations, therefore, we are going to follow the same procedure to obtain the formulations of necessary thermodynamic functions in the Heisenberg model

$$\hat{\mathcal{H}}_{ij}|n\rangle = E_n|n\rangle, \quad n = 1, 2, \dots, 10 \quad (4)$$

where $|n\rangle$ are the eigenvectors and E_n are the eigenvalues. Thus one has to consider the direct products of the possible vectors $|s_A, m_{s_A}\rangle_i$ for spin-2 and $|s_B, m_{s_B}\rangle_j$ for spin-1/2. As a result of the direct product, i.e. $|s_A, m_{s_A}\rangle_i \otimes |s_B, m_{s_B}\rangle_j$, one gets ten possible base vectors that are given as

$$\begin{aligned} |I\rangle &= |2, 2\rangle_i |1/2, 1/2\rangle_j, & |II\rangle &= |2, 2\rangle_i |1/2, -1/2\rangle_j, \\ |III\rangle &= |2, 1\rangle_i |1/2, 1/2\rangle_j, & |IV\rangle &= |2, 1\rangle_i |1/2, -1/2\rangle_j, \\ |V\rangle &= |2, 0\rangle_i |1/2, 1/2\rangle_j, & |VI\rangle &= |2, 0\rangle_i |1/2, -1/2\rangle_j, \\ |VII\rangle &= |2, -1\rangle_i |1/2, 1/2\rangle_j, & |VIII\rangle &= |2, -1\rangle_i |1/2, -1/2\rangle_j, \\ |IX\rangle &= |2, -2\rangle_i |1/2, 1/2\rangle_j, & |X\rangle &= |2, -2\rangle_i |1/2, -1/2\rangle_j \end{aligned} \quad (5)$$

which are used to obtain the matrix representation of the eigenvalue equation and where $\otimes$ is omitted for simplicity. Thus in this representation, one obtains 10×10 matrix whose elements are calculated from $E_{ij} = \langle i | \hat{\mathcal{H}}_{ij} | j \rangle$ with $i, j = I, II, \dots, X$. The non-zero elements are found as

$$\begin{aligned} E_{11} &= -J - 4D - 2h_i - h_j/2, & E_{22} &= J - 4D - 2h_i + h_j/2, \\ E_{33} &= -J/2 - D - h_i - h_j/2, & E_{44} &= J/2 - D - h_i + h_j/2, \\ E_{55} &= -h_j/2, & E_{66} &= h_j/2, \\ E_{77} &= J/2 - D + h_i - h_j/2, & E_{88} &= -J/2 - D + h_i + h_j/2, \\ E_{99} &= J - 4D + 2h_i - h_j/2, & E_{1010} &= -J - 4D + 2h_i + h_j/2, \\ E_{23} &= E_{32} = -J(1 - \Delta), & E_{45} &= E_{54} = -\sqrt{6}J(1 - \Delta)/2, \\ E_{67} &= E_{76} = -\sqrt{6}J(1 - \Delta)/2, & E_{89} &= E_{98} = -J(1 - \Delta). \end{aligned} \quad (6)$$

It is clear from the above matrix elements that the matrix representation of $\hat{\mathcal{H}}_{ij}$ in this base is symmetric. As a last step we need to find the eigenvalues and eigenvectors, i.e. correct superposition of the base vectors, of this matrix. Actually, the latter is not intended to be given in here, since we only need the eigenvalues to get our thermodynamic functions. The calculated eigenvalues are found as

$$\begin{aligned} E_{1,2} &= -4D \pm 2h_i \pm h_j/2 - J, \\ E_{3,4} &= [-10D + 6h_i + J \pm [36D^2 - 24Dh_i + 4h_i^2 + 24Dh_j - 8h_ih_j + 4h_j^2 - 36DJ \\ &\quad + 12h_iJ - 12h_jJ + 9J^2 + 64J'^2]^{1/2}]/4, \\ E_{5,6} &= [-10D - 6h_i + J \pm [36D^2 + 24Dh_i + 4h_i^2 - 24Dh_j - 8h_ih_j + 4h_j^2 - 36DJ \\ &\quad - 12h_iJ + 12h_jJ + 9J^2 + 64J'^2]^{1/2}]/4, \\ E_{7,8} &= [-4D - 4h_i + 2J \pm [(4D + 4h_i - 2J)^2 - 16(2Dh_j + 2h_ih_j - h_j^2 - h_iJ - 24J'^2)]^{1/2}]/8, \\ E_{9,10} &= [-4D + 4h_i + 2J \pm [(4D - 4h_i - 2J)^2 - 16(-2Dh_j + 2h_ih_j - h_j^2 + h_iJ - 24J'^2)]^{1/2}]/8 \end{aligned} \quad (7)$$

with $J' = \frac{1}{2}(1 - \Delta)$. They are used in the below equation to calculate the partition function

$$Z = \text{Tr}_{ij}[\exp(-\beta \hat{\mathcal{H}}_{ij})] = \sum_{i=1}^n e^{-\beta E_i} \quad (8)$$

with $\beta = 1/k_B T$ and k_B is the Boltzmann constant. In many statistical physics problems, the calculation of Z is the most important since all other thermodynamic functions can be calculated from it.

The magnetization and quadrupole moment for the sublattice A with spin-2 can be obtained from

$$M_A = \frac{1}{\beta Z} \frac{\partial Z}{\partial h_i} \quad (9)$$

and

$$Q_A = \frac{1}{\beta Z} \frac{\partial Z}{\partial D}. \quad (10)$$

Similarly, the magnetization for the sublattice B is calculated from

$$M_B = \frac{1}{\beta Z} \frac{\partial Z}{\partial h_j}. \quad (11)$$

The average magnetization can be defined as

$$M_T = (M_A + M_B)/2 \quad (12)$$

and the differences of sublattice magnetizations is defined as

$$M_C = |M_A - M_B| \quad (13)$$

which gives the compensation temperature when equals to zero. Finally, the free energy of the model can be obtained by using

$$F = -(1/\beta) \ln Z + J(z-1)M_A M_B. \quad (14)$$

It should be mentioned that the explicit forms of these equations are too long to be given in here. In order to obtain the numerical values of the order-parameters and free energy, an iteration procedure is followed by varying the temperatures for given system parameters. Thus the investigation of thermal variations of these quantities lead us to obtain the phase diagrams on possible planes spanned by the given system parameters.

Before presenting the phase diagrams of our model, the obtaining of second- and first-order phase transition and compensation temperatures and, critical points should be presented; (i) at the second-order phase transition temperature, T_c , the sublattice magnetizations go to zero continuously while the quadrupole moment makes a little kink, (ii) at the first-order phase transition temperature, T_t , the sublattice magnetizations present a jump to zero discontinuously where quadrupole moment also make a jump to some nonzero value, (iii) the compensation temperatures T_{comp} , which is caused by different responses of the sublattice magnetizations to temperature changes, can be calculated by obtaining the crossing points between the absolute values of the sublattice magnetizations

$$|M_A(T_{comp})| = |M_B(T_{comp})| \quad (15)$$

or when the net magnetization goes to zero, i.e.

$$M_{NET} = |M_A(T_{comp})| - |M_B(T_{comp})| = 0.0 \quad (16)$$

with the conditions

$$\text{sign}[M_A(T_{comp})] = -\text{sign}[M_B(T_{comp})], \quad T_{comp} < T_c. \quad (17)$$

Thus, these conditions warrant that the two sublattice magnetizations cancel each other at the compensation temperatures, (iv) the tricritical point (TCP) is defined as the juncture point of the T_c - and T_t -lines and (v) isolated critical points (ICP) are the points where the lines terminate. After presenting these important points, we are now ready to give our phase diagrams in the next section.

3. The phase diagrams

Before the illustrations of phase diagrams, we present the thermal variations of the order-parameters when they undergo second- or first-order phase transitions. Fig. 1a is obtained for $D/J = 1.0$ and $\Delta = 0.5$ shows the behaviors of order-parameters at the second-order phase transitions. As seen the magnetizations go to zero continuously at the same temperature, T_c , where Q_A makes a cusp exactly at the same temperature. The second one is obtained when $D/J = -2.8$ and $\Delta = 0.25$ which illustrates the existence of two first-order phase transitions. At these temperatures, T_t , the order-parameters present jump discontinuities. The next one shows the existence of a T_t and a T_c obtained for $D/J = -2.6$ and $\Delta = 0.25$. As seen the order-parameters first give a T_t than a T_c with $T_t < T_c$. The last one shows the thermal variations of M_c which shows the existence of two compensation temperatures obtained for $D/J = -2.75$ and $\Delta = 0.3$.

In the phase diagrams, the solid, dashed and dashed-dotted lines correspond to the second- and first-order phase transition and compensation temperatures, respectively. The filled triangles correspond to TCP's while the gray filled circles are used to indicate the ICP's of the T_t lines. The critical lines, T_c or T_t , at highest temperatures separate the paramagnetic phase regions (above the lines) from the ordered phase regions (below the lines). It should be noted that $\Delta = 1.0$ corresponds to mixed-spin Ising model, $\Delta = 0.0$ corresponds to the Heisenberg model called as XYZ model and for the intermediate values of Δ it is the exchange anisotropy included XYZ model.

The first phase diagrams of the mixed spin-2 and 1/2 model are obtained on the $(D/J, k_B T/J)$ planes for given values of Δ . Fig. 2a is calculated for $\Delta = 0.0$ shows that the critical line starts as a T_c -line at higher temperatures for higher D/J 's. This T_c -line terminates at a TCP, from where a small portion of T_t -line appears, then from the second TCP the other portion of the T_c -line is seen and it continues until very low negative D/J 's. In the Ising model the second portion does not appear at all. Actually this line disappear in the Ising models at about $D/J = 3.0$ at zero $k_B T/J$. The compensation line, T_{comp} -line, starts from the T_c -line and terminate on the lower portions of the T_t -lines. When $\Delta = 0.25$, see Fig. 2b, the T_t -line does not combine with the T_c -line at lower TCP instead it terminate at ICP. The second TCP combines the lower portion of the T_c -line with the triangular shaped T_t -line. Fig. 2c is obtained for $\Delta = 0.5$ is similar with the previous figure but now we see extra triangular shaped T_t -line. In all these figures, the T_{comp} -lines show reentrant behavior since the model gives two compensations. In addition, as Δ grows the portion of T_c -lines at lower negative D/J 's decrease as expected. Fig. 2d shows the phase diagram when $\Delta = 0.75$, it is clear that the T_c -line are seen at lower temperatures for lower D/J 's combine with a T_t -line at TCP which terminates at ICP. The T_{comp} -line terminate at the triangular shaped T_t -lines, then after a short break

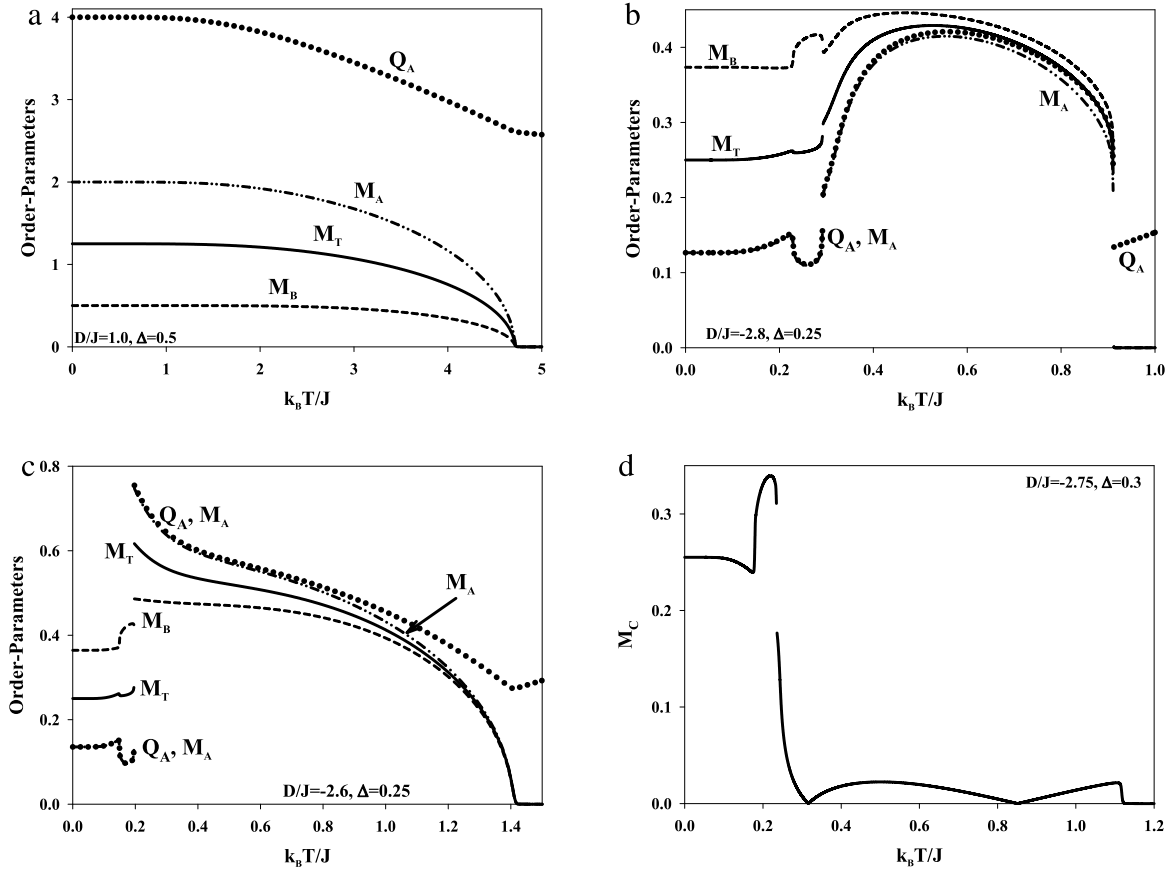


Fig. 1. The thermal variations of the order-parameters (a) $\Delta = 0.5$ and $D/J = 1.0$, (b) $\Delta = 0.25$ and $D/J = -2.8$, (c) $\Delta = 0.25$ and $D/J = -2.6$ and (d) the behavior of M_C showing two compensation temperatures when $\Delta = 0.3$ and $D/J = -2.75$.

it appears and then terminate at lower T_t . The last figure Fig. 2e corresponds to the Ising model, i.e. $\Delta = 1.0$. Except the triangular shaped T_t -line the phase diagram is very similar to the ones obtained in [9] of Fig. 4. In these phase diagrams, the lowest triangular shaped T_t -lines are unstable and all other lines are stable which can be easily seen from a free energy analysis. It should be mentioned that as Δ increases the increase in temperatures of T_c -lines almost unnoticeable.

The next ones are obtained on the $(\Delta, k_B T/J)$ planes for given values of D/J . Fig. 3a is obtained for the values of $D/J = 2.0, 1.5, 1.0, 0.5, 0.0, -0.5, -1.0, -1.5, -2.0$ and -2.4 . The T_c -lines decrease in temperature as D/J becomes smaller. They are almost straight for higher positive D/J , but they seem to go down in temperature as D/J becomes smaller at the $\Delta = 0.0$ side. Fig. 3b shows the case with $D/J = -2.5$ and -2.625 . Again the T_c -lines start from higher temperatures at $\Delta = 1.0$ and terminate at lower temperatures when $\Delta = 0.0$. The T_{comp} -line start from the T_c -line for $D/J = -2.625$ and terminates on the unstable portion of the T_t -lines and the reentrant behavior is also clear. A short T_{comp} -line starts from the $\Delta = 0.0$ for $D/J = -2.5$ and terminate on the T_t -lines. In Fig. 3c, the T_c -lines start from higher $k_B T/J$ and as Δ decrease the first TCP's appear for $D/J = -2.75$ and -2.8 , from where the T_t -lines start which then terminate at the lower TCP's. The T_{comp} -lines at $\Delta = 0.0$ and after showing reentrant behavior they terminate on their unstable T_t -lines. When $D/J = -2.9$, first we see a T_t -line ending at ICP, then a T_c -line starting from $\Delta = 0.0$ ending at the TCP, then the second T_t -line ending at the other ICP and a very low temperature T_t -line ending at ICP again. The T_{comp} -line again show reentrant behavior. Fig. 3e is similar to the previous figure, but now the lowest T_t -line is not seen. When $D/J = -3.0$, the temperature of T_t -line increase while it decrease when $D/J = -3.1$ towards $\Delta = 1.0$. The last figure is obtained when $D/J = -3.5, -4.0, -4.5, -5.0, -6.0, -8.0$ and -12.0 as shown in Fig. 3f. As seen the T_c -lines start from higher temperatures for $\Delta = 0.0$ and as Δ decreases their temperatures decrease and they terminate at TCP's of their own. The TCP's move to lower temperatures and higher Δ 's as D/J becomes more negative. The T_t -lines starting from TCP's terminate at zero temperatures close to $\Delta = 0.0$.

4. Brief summary and conclusions

In this work, we have tried to analyze mixed spin-2 and 1/2 Heisenberg model on a simple cubic lattice by using the OA. The exchange anisotropy and crystal field effects have been examined under the thermal changes. The phase diagrams are

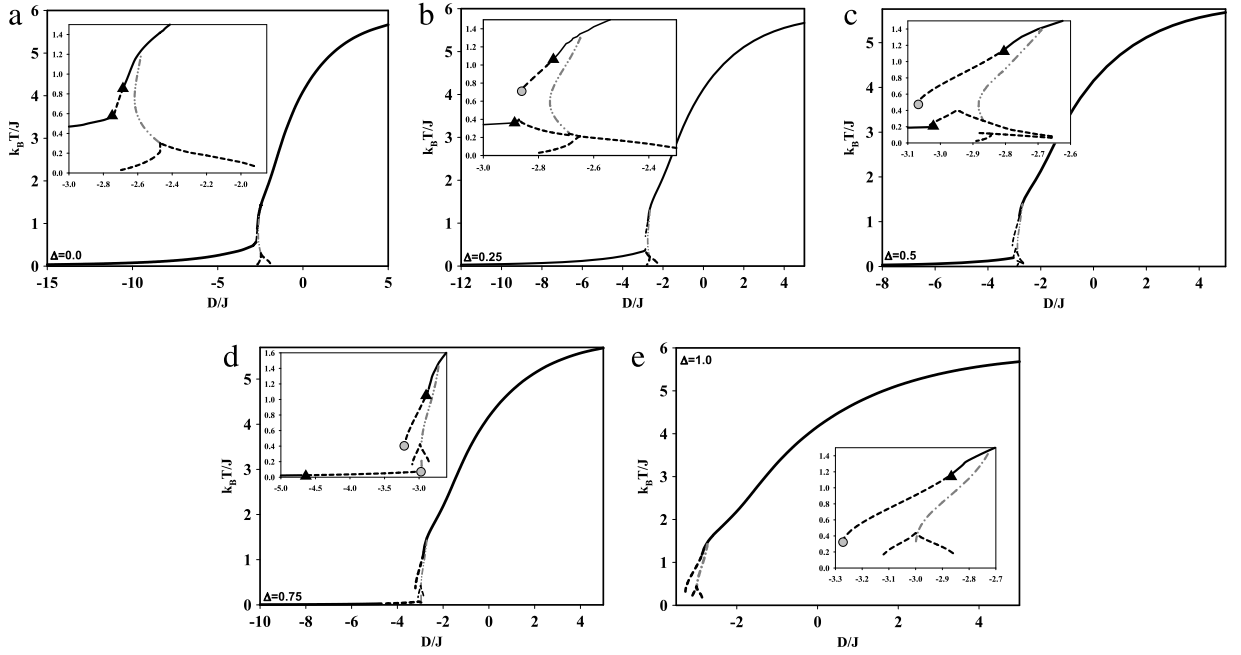


Fig. 2. The phase diagrams on the $(D/J, k_B T/J)$ planes for given values of Δ ; (a) 0.0, (b) 0.25, (c) 0.5, (d) 0.75 and (e) 1.0. The insets are intended to give all the details of the phase lines where the filled triangles and gray circles indicate the TCP's and ICP's, respectively.

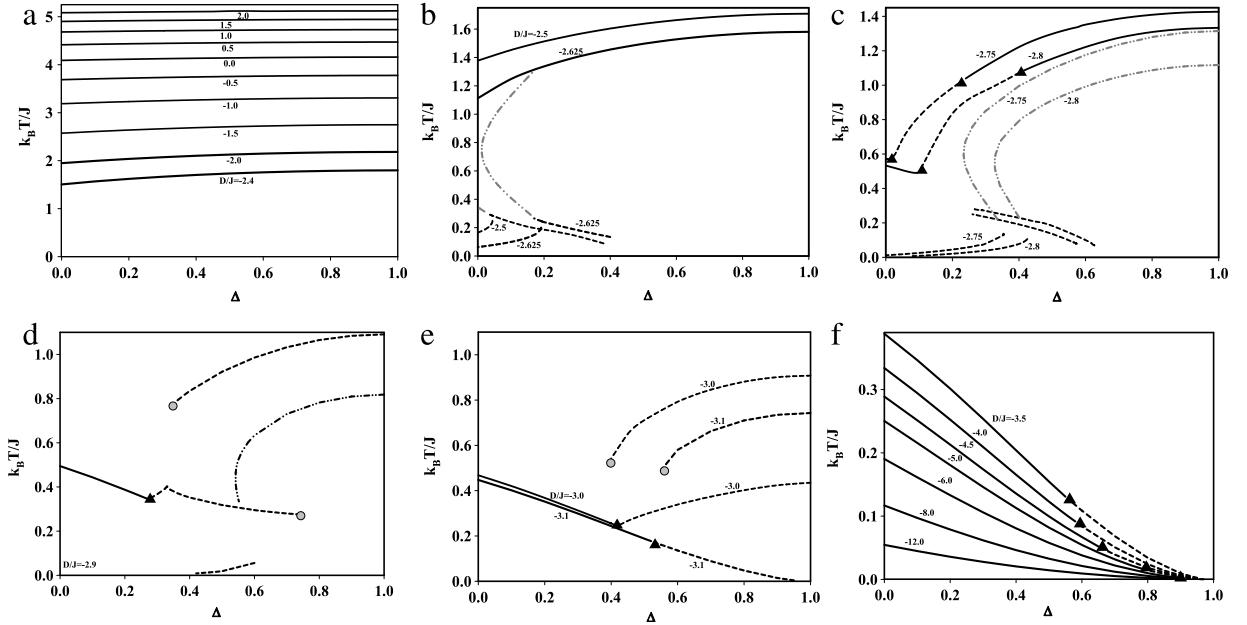


Fig. 3. The phase diagrams on the $(\Delta, k_B T/J)$ planes for given values of D/J ; (a) 2.0, 1.5, 1.0, 0.5, 0.0, -0.5 , -1.0 , -1.5 , -2.0 and -2.4 , (b) -2.5 and -2.625 , (c) -2.75 and -2.8 , (d) -2.9 , (e) -3.0 and -3.1 and (f) -3.5 , -4.0 , -4.5 , -5.0 , -6.0 , -8.0 and -12.0 .

calculated by studying the thermal changes of the order-parameters and free energy. In addition to the stable solutions, the unstable solutions of the model are also examined. The model yields both second- and first-order transitions, in addition to the TCP and ICP. The compensation temperatures are found which led to the reentrant behavior. Some important conclusions are given during the explanations of figures and whenever possible a few comparisons are also made and similarities are observed. As an important conclusion, even if this mixed-spin system including anisotropy is not studied with any other techniques so far, we see for the case with $\Delta = 1.0$, i.e. [8–11], some shortcomings or maybe some kinds of artifacts at low temperature regions.

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ANISOTROPIC HEISENBERG MODEL FOR THE MIXED SPIN-2 AND SPIN-1/2 IN THE OGUCHI APPROXIMATION ON SQUARE AND SIMPLE CUBIC LATTICES

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The mixed spin-2 and spin-1/2 Heisenberg model is studied on square and simple cubic lattices by using the Oguchi approximation to examine the effects of exchange anisotropy and crystal field. The thermal variations order-parameters, i.e. magnetization and quadrupole moment, are investigated to obtain the possible phase diagrams of the model. The detailed phase diagrams are obtained on the $(D/J, kBT/J)$ and $(\Delta, kBT/J)$ planes for given values of Δ and D/J , respectively. In the phase diagrams all possible solutions are illustrated whether stable or not. The model yields second and first-order phase transitions, in addition to the tricritical and isolated critical points. The model also gives two compensation temperatures for given system parameters, therefore, they exhibit reentrant behavior. The low temperature behavior of the model is very complicated, therefore, the reliability of the Oguchi approximation should be investigated further.

CRITICAL PHASE BEHAVIOURS UNDER THE NEGATIVE PRESSURE OF THE POLYMER SOLUTIONS AT AND NEAR THE MATHEMATICAL DOUBLE POINTS*

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We investigate the critical lines and global phase behavior of polymer solutions at the mathematical double point (MDP) and its vicinity by using Flory-Huggins Tompa model, for positive and under the negative pressure. A principal transition mechanism is a MDP at which two critical lines meet and exchange branches. We present the global phase diagrams in the density-density, pressure-temperature and temperature density planes. We found that as the chain length increases, the MDP shifts to the low pressure region and is found in the negative pressure region when the chain length factor $r = 20$. Also we found that our results correspond to the phase transition from inverse type II to inverse type III, from inverse type II to inverse type III through inverse type IV under the negative pressure region.

* Erciyes Üniversitesi Araştırma Fonu (No: FYL-2017-7256) tarafından desteklenmiştir.

STATISTICAL PHYSICS

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RAPOR

Bu projede, karma spin-2 ve spin-1/2 Hesienberg modelinde deęiş-tokuş enerjisi ve kristal alan etkileri Oguchi yaklaşımı kullanılarak kare ve basit kübik kafes üzerinde detaylıca çalışıldı. Düzen parametrelerinin, manyetik dipol ve kuadrupol moment, ve serbest enerjinin sıcaklıkla olan deęişimleri incelenerek sistemin mümkün olan düzlemlerdeki faz diyagramları elde edildi. Detaylı faz diyagramları (D/J , $k_B T/J$) ve (Δ , $k_B T/J$) düzlemlerinde sırasıyla verilen Δ ve D/J deęerleri için elde edilip faz diyagramlarında kararlı ya da kararsız olsun bütün çözümler gösterildi. Modelin üçlü kritik ve izole edilmiş kritik noktaların yanı sıra ikinci- ve birinci seviye faz geçişleri verdiği bulundu. Model aynı zamanda verilmiş sistem parametreleri için iki telafi (compensation) sıcaklığı vermiştir ki buda reentrant olayına sebebiyet vermiştir. Modelin düşük sıcaklık bölgesindeki davranışı çok karmaşıktır ki bundan dolayı bu modelin güvenilirliğinin tespiti daha ileri seviyede incelenmesi gereklidir. Elde ettiğimiz sonuçlar literatürde bulunan çalışmalarla benzer sonuçlar vermesinin yanı sıra Heisenberg modelinde kullanılan Oguchi yaklaşımının yeterli ve yetersiz yanlarını da ortaya çıkarmıştır. Yapılan çalışmalarımız ile hedeflediğimiz bilimsel sonuçlara ulaşmanın yanı sıra uluslararası Science Citation Index (SCI) iki adet yayın [14,15] ve uluslararası bir adet sözlü sunum [16] yapılmıştır ki bu hedef proje başvurusunda belirtilmişti.

Bu projenin 8157,99 TL olan bütçesinin 4788,44 TL'lik kısmı dizüstü bilgisayar, 895,62 TL'lik kısmı monitör ve 1822,96 TL'lik kısmı ise uluslararası sunum yapmak üzere toplam 7505.02 TL'lik kısmı kullanılmış olup geri kalan kısmı olan 650.97 TL'lik kısmı ise kullanılmamıştır.

Ekler: 1-Makale [14] ve Makale [15]

2- Uluslararası Sözlü Bildiri