Onsager reaction-field theory for magnetic models on diamond and hcp lattices

G. M. Wysin
Department of Physics, Kansas State University, Manhattan, Kansas 66506-2601
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The Onsager reaction-field (ORF) theory is extended to apply to three-dimensional Bravais lattices with a basis. The ORF calculation is used to predict the critical temperature for classical Ising, *XY*, and Heisenberg magnetic models, in particular, on diamond and hexagonal close-packed lattices. Results are compared with series extrapolations and other theoretical approaches where available. For the hcp lattice the ORF calculation is seen to be equivalent to a Green's-function approach by Adler [Physica B&C **107B**, 207 (1981)].

I. INTRODUCTION

The Onsager reaction field (ORF) theory[1] is an improved form of mean-field theory that includes at least partially the effects of correlations between nearby atoms. It was originally applied in magnetism by Brout and Thomas,[2] and more recently to spin glasses,[3] itinerant electron systems,[4] Hubbard models,[5] and anisotropic Heisenberg[6] and *XY* (Ref. 7) models. The procedure is versatile and has been used to estimate specific heat, susceptibility, and correlations above the critical temperature T_c, as well as T_c itself. A clear review of the ORF method applied to three-dimensional (3D) Ising models is given by White.[8] The method has been applied on the standard Bravais lattices, including simple cubic (sc), body-centered cubic (bcc), and face-centered cubic (fcc), with results given in terms of integrals over the associated Brillouin zone (BZ). However, a modification of these calculations is needed to consider other lattices which are not in the Bravais classification. Here we show how to apply the ORF procedure to any non-Bravais lattice that can be considered as an underlying Bravais lattice with a basis. In particular, the diamond and hexagonal close-packed lattices are analyzed, both of which have two-atom bases.

In the usual mean field theory due to Weiss,[9] a chosen atom (or spin, for the magnetic problems we consider) is viewed as interacting with the average, or mean field, of its nearest neighbors. The exact Hamiltonian is replaced by the mean field one, in which the neighbors are introduced as the mean-field acting on the central atom. However, the central atom itself influences the neighbors, and therefore the mean-field usually includes a part directly attributed to the central atom. This means the mean-field includes a part that might be considered a self-interaction effect, which should really be subtracted out. This results in an overestimate of the critical temperature T_c. The ORF procedure is simply a way to estimate and subtract out this self-interaction part, i.e., by adding a ''reaction field'' term that accomplishes this. In this way, the estimate of T_c is brought down, indeed, usually ORF leads to an underestimate of T_c.

The standard ORF approach uses as input the specific lattice structure, be it sc, fcc, bcc, etc. However, the usual approach and well-known formulas require the perfect periodicity of a Bravais lattice—all atoms are taken as equivalent. On the other hand, we have been interested in mean field and other calculations[10] for diamond lattices because of the low coordination number ($z=4$). The diamond lattice is not a Bravais lattice—all sites do not have the same surroundings, instead, the diamond lattice can be considered to be a fcc lattice with a two atom basis. Thus it is interesting to understand how to apply the ORF procedure to such a system.

Recently there also is interest in ferromagnetic ordering of hcp ^{3}He at low temperatures,[11] assumed to be described by a Heisenberg model. The hcp lattice with Ising variables has also been considered as a model for roughening transitions on ^{4}He crystals.[12] The hcp lattice is another non-Bravais lattice; it can be considered as simple hexagonal (stacked triangular nets), also with a two-atom basis. A simple analysis procedure such as ORF applied to the hcp system, including the possibility of anisotropic exchange interactions, may be useful for the interpretation of He experiments at low temperature. Here we show how to extend the standard ORF calculation of T_c to these two systems, however, our approach will apply to any Bravais lattice with a basis, i.e., any system with multiple atoms per unit cell.

II. MODEL AND REACTION FIELD

For simplicity we display formulas for Ising models on a 3D lattice with spins $S_n=\pm S$ and coordination number z. However, the modifications to treat n-component spins [i.e., *XY* ($n=2$), Heisenberg ($n=3$), etc.] are minimal and will be noted where they are appropriate. The Hamiltonian is

$$\mathcal{H}_0=-\frac{1}{2}\sum_{\mathbf{n}}\sum_{\mathbf{m}} J_{\mathbf{n},\mathbf{m}}S_{\mathbf{n}}S_{\mathbf{m}}-\sum_{\mathbf{n}} H_{\mathbf{n}}S_{\mathbf{n}}, \tag{1}$$

where each sum is over all of the lattice sites, and the bond coupling strength $J_{\mathbf{n},\mathbf{m}}$ depends only on the neighbor displacement, $\mathbf{n}-\mathbf{m}$, and is of the same strength J for all near-neighbor pairs. The factor of $\frac{1}{2}$ cancels the double counting of bonds, and $H_{\mathbf{n}}$ is a spatially varying applied field.

In the ORF calculation (see Ref. 8 for more details), a spin at a chosen site interacts with the mean-field reduced by a ''reaction field'' that depends on the spin at that site.[1] In the real-space Hamiltonian the reaction term is an extra self-interaction:

$$\mathcal{H}_{\rm rf}=\lambda\sum_{\mathbf{n}} S_{\mathbf{n}}S_{\mathbf{n}}. \tag{2}$$

This is equivalently a delta-function exchange term of strength λ. The constant λ is the reaction field, which is determined self-consistently in the calculation, by a constraint on the magnetic susceptibility, below.

III. ORF THEORY FOR BRAVAIS LATTICES WITH A BASIS

We suppose that the lattice has an underlying set of N Bravais lattice points $\mathbf{n}$, each of which has a two-atom basis $\{\mathbf{0},\mathbf{d}\}$. (The generalization to a larger basis is straightforward.) At each site $\mathbf{n}$ there is a double spin field $\tilde{S}_{\mathbf{n}}$ written as a column vector:

$$\tilde{S}_{\mathbf{n}}=\begin{pmatrix} S_{\mathbf{n}}^{(1)} \\ S_{\mathbf{n}}^{(2)} \end{pmatrix}=\begin{pmatrix} S_{\mathbf{n}} \\ S_{\mathbf{n}+\mathbf{d}} \end{pmatrix}, \tag{3}$$

where the superscripts on $S_{\mathbf{n}}$ label the spins on the two separate sublattices, and we use tildes to indicate matrix quantities. The exchange interaction occurs between neighboring Bravais sites, via a 2×2 matrix, $\tilde{J}_{\mathbf{n},\mathbf{m}}$:

$$\mathcal{H}_{\mathrm{ex}}=-\frac{1}{2}\sum_{\mathbf{n}}\sum_{\mathbf{m}}\tilde{S}_{\mathbf{n}}^{T}\cdot\tilde{J}_{\mathbf{n},\mathbf{m}}\cdot\tilde{S}_{\mathbf{m}}, \tag{4}$$

where it is stressed that the sums are over all Bravais sites; the factor of $\frac{1}{2}$ cancels the double counting of bonds, and

$$\tilde{J}_{\mathbf{n},\mathbf{m}}=\begin{pmatrix} J^{11} & J^{12} \\ J^{21} & J^{22} \end{pmatrix}_{\mathbf{n},\mathbf{m}}=\begin{pmatrix} J_{\mathbf{n},\mathbf{m}} & J_{\mathbf{n},\mathbf{m}+\mathbf{d}} \\ J_{\mathbf{n}+\mathbf{d},\mathbf{m}} & J_{\mathbf{n}+\mathbf{d},\mathbf{m}+\mathbf{d}} \end{pmatrix}. \tag{5}$$

In fact, the matrix $\tilde{J}_{\mathbf{n},\mathbf{m}}$ is taken as zero unless $\mathbf{n}-\mathbf{m}$ is a near-neighbor displacement. The details of the specific lattice will determine which components of $\tilde{J}$ are nonzero.

The reaction terms, two for each site $\mathbf{n}$, can be written with a 2×2 unit matrix $\tilde{\mathcal{I}}$,

$$\mathcal{H}_{\mathrm{rf}}=\frac{1}{2}\sum_{\mathbf{n}}\sum_{\mathbf{m}}\tilde{S}_{\mathbf{n}}^{T}\cdot[2\lambda\,\delta_{n,m}\tilde{\mathcal{I}}]\cdot\tilde{S}_{\mathbf{m}}, \tag{6}$$

which is equivalent to expression (2), and essentially shifts the original exchange matrix by $-2\lambda\,\delta_{n,m}\tilde{\mathcal{I}}$.

Finally, for the purpose of the calculation, there is a separate applied field for each sublattice, so at a given site $\mathbf{n}$, we have fields $H_{\mathbf{n}}^{(1)}$ (acting on $S_{\mathbf{n}}$) and $H_{\mathbf{n}}^{(2)}$ (acting on $S_{\mathbf{n}+\mathbf{d}}$). These compose a column vector field,

$$\tilde{H}_{\mathbf{n}}=\begin{pmatrix} H_{\mathbf{n}}^{(1)} \\ H_{\mathbf{n}}^{(2)} \end{pmatrix}. \tag{7}$$

It is convenient to transform into Fourier space, according to

$$\tilde{S}_{\mathbf{n}}=\frac{1}{\sqrt{N}}\sum_{\mathbf{q}}\tilde{S}_{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{n}}, \tag{8}$$

$$\tilde{J}_{\mathbf{n},\mathbf{m}}=\frac{1}{N}\sum_{\mathbf{q}}\tilde{J}_{\mathbf{q}}e^{i\mathbf{q}\cdot(\mathbf{n}-\mathbf{m})}. \tag{9}$$

There is a relation similar to Eq. (8) for the Fourier-transformed applied field $\tilde{H}_{\mathbf{q}}=\tilde{H}_{-\mathbf{q}}$. The Fourier-transformed exchange interaction is

$$\tilde{J}_{\mathbf{q}}=\sum_{\mathbf{r}}\tilde{J}_{\mathbf{r}}e^{i\mathbf{q}\cdot\mathbf{r}}, \tag{10}$$

i.e., a sum over displacements to nearest neighbors, $\mathbf{r}\equiv\mathbf{m}-\mathbf{n}$. Then we write the q-space Hamiltonian, including the reaction term and applied fields, as

$$\mathcal{H}=-\frac{1}{2}\sum_{\mathbf{q}}[\tilde{S}_{-\mathbf{q}}^{T}\cdot(\tilde{J}_{\mathbf{q}}-2\lambda\tilde{\mathcal{I}})\cdot\tilde{S}_{\mathbf{q}}+(\tilde{S}_{-\mathbf{q}}^{T}\cdot\tilde{H}_{\mathbf{q}}+\tilde{S}_{\mathbf{q}}^{T}\cdot\tilde{H}_{-\mathbf{q}})]. \tag{11}$$

The factor of 2 on λ corresponds to the two-atom basis. This Hamiltonian is exact.

Now we consider the mean-field approximation in q space, i.e., using a random-phase approximation (RPA), magnetization components at different wave vectors are assumed to be independent. From the point of view of the negative-q components, the Hamiltonian is approximated as

$$\mathcal{H}=-\sum_{\mathbf{q}}\tilde{S}_{-\mathbf{q}}^{T}\cdot[\tilde{H}_{\mathbf{q}}+\tilde{K}_{\mathbf{q}}\cdot\langle\tilde{S}_{\mathbf{q}}\rangle], \tag{12}$$

where we use the shorthand notation for the shifted exchange interaction,

$$\tilde{K}_{\mathbf{q}}\equiv\tilde{J}_{\mathbf{q}}-2\lambda\tilde{\mathcal{I}}. \tag{13}$$

The above Hamiltonian can alternatively be written in terms of effective fields $H_{\mathbf{q}}^{\mathrm{e}}$, in components,

$$\mathcal{H}=-\sum_{\mathbf{q}}[H_{\mathbf{q}}^{\mathrm{e}(1)}S_{-\mathbf{q}}^{(1)}+H_{\mathbf{q}}^{\mathrm{e}(2)}S_{-\mathbf{q}}^{(2)}], \tag{14}$$

$$H_{\mathbf{q}}^{\mathrm{e}(1)}=H_{\mathbf{q}}^{(1)}+K_{\mathbf{q}}^{11}\langle S_{\mathbf{q}}^{(1)}\rangle+K_{\mathbf{q}}^{12}\langle S_{\mathbf{q}}^{(2)}\rangle, \tag{15a}$$

$$H_{\mathbf{q}}^{\mathrm{e}(2)}=H_{\mathbf{q}}^{(2)}+K_{\mathbf{q}}^{21}\langle S_{\mathbf{q}}^{(1)}\rangle+K_{\mathbf{q}}^{22}\langle S_{\mathbf{q}}^{(2)}\rangle. \tag{15b}$$

In the ORF approach, T_c is found by locating the singular point of the magnetic susceptibility. Therefore we define the sublattice magnetizations ($i=1,2$),

$$M_{\mathbf{q}}^{i}=\langle S_{\mathbf{q}}^{i}\rangle, \tag{16}$$

and related zero-field susceptibilities,

$$\chi_{\mathbf{q}}^{ij}=\frac{\partial M_{\mathbf{q}}^{i}}{\partial H_{\mathbf{q}}^{j}}=\beta\langle S_{\mathbf{q}}^{i}S_{-\mathbf{q}}^{j}\rangle. \tag{17}$$

Using the RPA Hamiltonian (14), the susceptibility definitions become

$$\chi_{\mathbf{q}}^{ij}=\frac{\partial M_{\mathbf{q}}^{i}}{\partial H_{\mathbf{q}}^{\mathrm{e}i}}\frac{\partial H_{\mathbf{q}}^{\mathrm{e}i}}{\partial H_{\mathbf{q}}^{j}}, \tag{18}$$

and we get equations for the susceptibility components,

$$\chi_{\mathbf{q}}^{11}=\beta\langle S_{\mathbf{q}}^{(1)}S_{-\mathbf{q}}^{(1)}\rangle_0[1+K_{\mathbf{q}}^{11}\chi_{\mathbf{q}}^{11}+K_{\mathbf{q}}^{12}\chi_{\mathbf{q}}^{21}], \tag{19a}$$

$$\chi_{\mathbf{q}}^{12}=\beta\langle S_{\mathbf{q}}^{(1)}S_{-\mathbf{q}}^{(1)}\rangle_0[K_{\mathbf{q}}^{11}\chi_{\mathbf{q}}^{12}+K_{\mathbf{q}}^{12}\chi_{\mathbf{q}}^{22}], \tag{19b}$$

$$\chi_{\mathbf{q}}^{22}=\beta\langle S_{\mathbf{q}}^{(2)}S_{-\mathbf{q}}^{(2)}\rangle_0[1+K_{\mathbf{q}}^{22}\chi_{\mathbf{q}}^{22}+K_{\mathbf{q}}^{21}\chi_{\mathbf{q}}^{12}], \tag{19c}$$

$$\chi_{\mathbf{q}}^{21}=\beta\langle S_{\mathbf{q}}^{(2)}S_{-\mathbf{q}}^{(2)}\rangle_0[K_{\mathbf{q}}^{22}\chi_{\mathbf{q}}^{21}+K_{\mathbf{q}}^{21}\chi_{\mathbf{q}}^{11}], \tag{19d}$$

where $\langle\ \rangle_0$ means the expectation value using the RPA Hamiltonian. In the high-temperature limit, these expectations are

$$\beta\langle S_{\mathbf{q}}^{(1)}S_{-\mathbf{q}}^{(1)}\rangle_0=\beta\langle S_{\mathbf{q}}^{(2)}S_{-\mathbf{q}}^{(2)}\rangle_0=\frac{\beta}{n}S^2\equiv\chi_0. \tag{20}$$

Equations (19) can be solved in the general case for all four susceptibility components. We get

$$\chi_{\mathbf{q}}^{11}=\chi_0\frac{1-\chi_0K_{\mathbf{q}}^{22}}{(1-\chi_0K_{\mathbf{q}}^{11})(1-\chi_0K_{\mathbf{q}}^{22})-\chi_0^2K_{\mathbf{q}}^{12}K_{\mathbf{q}}^{21}}, \tag{21a}$$

$$\chi_{\mathbf{q}}^{21}=\chi_0\frac{K_{\mathbf{q}}^{21}\chi_{\mathbf{q}}^{11}}{1-\chi_0K_{\mathbf{q}}^{22}}, \tag{21b}$$

and similar equations for $\chi_{\mathbf{q}}^{22}$ and $\chi_{\mathbf{q}}^{12}$ by appropriately interchanging the indices. For the lattices considered in this paper, however, there are the symmetries, $K_{\mathbf{q}}^{11}=K_{\mathbf{q}}^{22}$ and $K_{\mathbf{q}}^{12}=(K_{\mathbf{q}}^{21})^*$. Therefore the solutions are seen to satisfy symmetries $\chi_{\mathbf{q}}^{11}=\chi_{\mathbf{q}}^{22}$, $\chi_{\mathbf{q}}^{12}=(\chi_{\mathbf{q}}^{21})^*$.

Now consider how to determine the reaction field λ, and subsequently, T_c. Using the definitions of $\chi_{\mathbf{q}}^{11}$ and $S_{\mathbf{q}}^{(1)}$, shows that there is the constraint,

$$\frac{1}{N}\sum_{\mathbf{q}}\chi_{\mathbf{q}}^{11}=\frac{\beta}{n}S^2\equiv\chi_0. \tag{22}$$

This equation implicitly determines the reaction coupling λ for any $T>T_c$. It is not clear how to get an explicit solution for λ from it; a solution for $\lambda(T)$ for a given lattice can be found numerically (below).

The critical temperature T_c is the temperature at which any of the susceptibility components, at $\mathbf{q}=\mathbf{0}$, diverges. The $\chi_{\mathbf{q}}^{ij}$ are well defined on the high-temperature side of T_c. For temperatures below T_c the ORF calculation gives negative susceptibility at $\mathbf{q}=\mathbf{0}$, signifying the presence of the ordered state. So T_c is determined as the point at which the denominator of Eq. (21a) goes to zero, leading to a relation between the critical temperature (via χ_0) and the critical reaction field,

$$\chi_0^{-1}+2\lambda=J_0^{11}+\sqrt{J_0^{12}J_0^{21}}. \tag{23}$$

Using this in the constraint Eq. (22) together with the result (21a) for $\chi_{\mathbf{q}}^{11}$, gives the general result when the symmetry $J_{\mathbf{q}}^{11}=J_{\mathbf{q}}^{22}$ holds,

$$k_BT_c=\frac{J_0S^2}{nI}, \tag{24a}$$

$$I=\frac{1}{N}\sum_{\mathbf{q}}\frac{J_0(J_0-J_{\mathbf{q}}^{11})}{(J_0-J_{\mathbf{q}}^{11})^2-J_{\mathbf{q}}^{12}J_{\mathbf{q}}^{21}}, \tag{24b}$$

where J_0 is the effective $\mathbf{q}=\mathbf{0}$ exchange strength,

$$J_0\equiv J_0^{11}+\sqrt{J_0^{12}J_0^{21}}. \tag{25}$$

The sum I defined in this way again gives the correction to the mean-field prediction for T_c. The sum (24b) can also be expressed in the alternative form,

$$I=\frac{1}{2N}\sum_{\mathbf{q}}\left[\frac{J_0}{J_0-J_{\mathbf{q}}^{11}+\sqrt{J_{\mathbf{q}}^{12}}}+\frac{J_0}{J_0-J_{\mathbf{q}}^{11}-\sqrt{J_{\mathbf{q}}^{12}}}\right]. \tag{26}$$

The above result (24) also applies to Bravais lattices, where the exchange matrix has only one element, $J_{\mathbf{q}}$, giving the familiar result[8]

$$I=\frac{1}{N}\sum_{\mathbf{q}}\frac{J_0}{J_0-J_{\mathbf{q}}}. \tag{27}$$

In the continuum limit, $(1/N)\Sigma\mathbf{q}\rightarrow(V/N)\int d^3q/(2\pi)^3$, where V/N is the specific volume per lattice site. For example, $V/N=a^3,\frac{1}{2}a^3,\frac{1}{4}a^3$ for sc, bcc, and fcc lattices, respectively, where a^3 is the cubic unit-cell volume. At $\mathbf{q}=\mathbf{0}$ we have $J_0=zJ$, which gives the energy scale in the mean-field approximation. From integration over the appropriate Brillouin zones, the values of I are 1.516, 1.393, and 1.345 for sc, bcc, and fcc lattices, respectively.[15] When applied to the 3D Ising model ($n=1$) one gets $k_BT_c/JS^2=z/I=3.957,5.742,8.924$ for sc, bcc, and fcc lattices, considerable improvements over the standard mean-field results given from $k_BT_c/JS^2=z$. These compare favorably with the exact Ising model results[13,14] from series: $k_BT_c/JS^2=4.5103,6.3508,9.794$, respectively. For the Heisenberg model ($n=3$), the ORF predicts $k_BT_c/JS^2=1.319,1.914$, for sc and bcc lattices, whereas precise Monte Carlo estimates[16] give $k_BT_c/JS^2=1.443,2.054$, respectively. Generally, the ORF estimates are all below the exact results.

It is also possible to compare with the results of a Green's-function approach[17] with RPA for the quantum Heisenberg model,[18] where Eq. (24) is replaced by

$$k_BT_c=\frac{J_0S(S+1)}{3I}, \tag{28}$$

with I given by Eq. (27), i.e., the *same* as the classical values. Therefore, at large S, the correction to the mean-field T_c is the same factor I for the RPA applied via the quantum Green's-function approach as it is for the classical ORF approach.

Below we will use Eq. (24) to estimate the critical temperature for diamond and hcp lattices. But first we verify that the result is correct by using it for a bcc lattice, considered as a simple-cubic lattice with a basis, where we already know the standard ORF result for T_c.

IV. BCC LATTICE AS SC WITH BASIS

The bcc lattice points can be generated from the simple cubic primitive vectors, $\mathbf{a}_1=a\hat{x}$, $\mathbf{a}_2=a\hat{y}$, and $\mathbf{a}_3=a\hat{z}$, where a is the cubic cell lattice constant, together with the basis, $\{\mathbf{0},\mathbf{d}\}$, where $\mathbf{d}=(a/2)(\hat{x}+\hat{y}+\hat{z})$ is the displacement to the body-centered point. The lattice can be thought of as a pair of interpenetrating sc lattices (sublattices 1 and 2) with displacement $\mathbf{d}$. The near neighbors of a '1' site are all ''2''

sites, and vice versa, with the result that the J^{11} and J^{22} couplings are all zero. The nonzero $J^{ij}_{\mathbf{n},\mathbf{m}} \equiv J^{ij}_{\mathbf{r}}$ couplings depend only on the near-neighbor displacement, $\mathbf{r} \equiv \mathbf{m} - \mathbf{n}$, as follows:

$$J^{21}_{\mathbf{r}} = J^{12}_{-\mathbf{r}} = J, \mathbf{r} = \{\mathbf{0}, \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3, \mathbf{a}_1 + \mathbf{a}_2, \mathbf{a}_2 + \mathbf{a}_3, \mathbf{a}_3 + \mathbf{a}_1\}, \tag{29}$$

where the terms for $\mathbf{r} = \mathbf{0}$ correspond to the coupling within the two-atom basis. The fact that $J^{11}_{\mathbf{n},\mathbf{m}} = J^{22}_{\mathbf{n},\mathbf{m}} = 0$ simplifies the determination of T_c considerably, as we only need to know the product, $J^{12}_{\mathbf{q}} J^{21}_{\mathbf{q}}$.

The Fourier-transformed interactions are found to be

$$J^{12}_{\mathbf{q}} = \sum_{\mathbf{r}} J^{12}_{\mathbf{r}} e^{i\mathbf{q}\cdot\mathbf{r}} = (J^{21}_{\mathbf{q}})^*, \tag{30}$$

$$J^{12}_{\mathbf{q}} = J\{1 + e^{-iq_x} + e^{-iq_y} + e^{-iq_z} + e^{-i(q_x+q_y)} + e^{-i(q_y+q_z)} + e^{-i(q_z+q_x)} + e^{-i(q_x+q_y+q_z)}\}. \tag{31}$$

In this and the following equations, q_x, q_y, q_z are in units of $1/a$. For the underlying sc lattice, the density of points is 1 for every volume a^3, i.e., $V/N = a^3$. After a short calculation, there results

$$J^{12}_{\mathbf{q}} J^{21}_{\mathbf{q}} = 8J^2\{1 + \cos q_x + \cos q_y + \cos q_z + \cos q_x \cos q_y + \cos q_y \cos q_z + \cos q_z \cos q_x + \cos q_x \cos q_y \cos q_z\}, \tag{32}$$

and the determination of T_c relies on evaluation of the simplified integral,

$$I = \frac{1}{(2\pi)^3} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{dq_x dq_y dq_z}{1 - J^{12}_{\mathbf{q}} J^{21}_{\mathbf{q}} / J_0^2}, \tag{33}$$

where $J_0 = J^{12}_{\mathbf{0}} = J^{21}_{\mathbf{0}} = 8J = zJ$. The integral can be rewritten using the periodicity and symmetry in q space, together with variable change $\mathbf{q}/2 \rightarrow \mathbf{q}$, as

$$I = \frac{1}{(2\pi)^3} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{dq_x dq_y dq_z}{1 - \cos q_x \cos q_y \cos q_z}. \tag{34}$$

The integral has been evaluated by Watson[15] to be $I = 1.393\,20\ldots$. Therefore the estimate of the critical temperature that results is

$$k_B T_c = \frac{8JS^2}{n} \frac{1}{1.393\,20} = \frac{5.742\,18}{n} JS^2, \tag{35}$$

in exact agreement with the result from Eq. (27).

V. DIAMOND LATTICE

The diamond lattice can be considered as an fcc lattice with a two-atom basis, i.e., sublattices 1 and 2. The fcc primitive vectors are $\mathbf{a}_1 = (a/2)(\hat{x} + \hat{y}), \mathbf{a}_2 = (a/2)(\hat{y} + \hat{z}), \mathbf{a}_2 = (a/2)(\hat{z} + \hat{x})$, where a is the standard cubic cell lattice constant, and the basis is $\{\mathbf{0}, \mathbf{d}\}$, where $\mathbf{d} = (a/4)(\hat{x} + \hat{y} + \hat{z})$. The nearest neighbors of a site $\mathbf{n} + \mathbf{d}$ (a 2-site) are $\{\mathbf{n}, \mathbf{n} + \mathbf{a}_1, \mathbf{n} + \mathbf{a}_2, \mathbf{n} + \mathbf{a}_3\}$ (all 1 sites). The nearest neighbors of a site $\mathbf{n}$ (a 1 site) are at $\{\mathbf{n} + \mathbf{d}, \mathbf{n} + \mathbf{d} - \mathbf{a}_1, \mathbf{n} + \mathbf{d} - \mathbf{a}_2, \mathbf{n} + \mathbf{d} - \mathbf{a}_3\}$ (all 2 sites). As a result, only J^{12} and J^{21} are nonzero. In terms of the neighbor displacements $\mathbf{r} = \mathbf{m} - \mathbf{n}$, the only nonzero exchange couplings are

$$J^{21}_{\mathbf{r}} = J^{12}_{-\mathbf{r}} = J, \mathbf{r} = \{\mathbf{0}, \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}. \tag{36}$$

Then it is straightforward to evaluate

$$J^{12}_{\mathbf{q}} = \sum_{\mathbf{r}} J^{12}_{\mathbf{r}} e^{i\mathbf{q}\cdot\mathbf{r}} = (J^{21}_{\mathbf{q}})^* \tag{37a}$$

$$= J[1 + e^{-i\mathbf{q}\cdot\mathbf{a}_1} + e^{-i\mathbf{q}\cdot\mathbf{a}_2} + e^{-i\mathbf{q}\cdot\mathbf{a}_3}], \tag{37b}$$

and what is needed for the T_c integral:

$$J^{12}_{\mathbf{q}} J^{21}_{\mathbf{q}} = 4J^2\left[1 + \cos\frac{q_x}{2}\cos\frac{q_y}{2} + \cos\frac{q_y}{2}\cos\frac{q_z}{2} + \cos\frac{q_z}{2}\cos\frac{q_x}{2}\right], \tag{38}$$

where q's are in units of $1/a$. Clearly we also have once again, $J_0 = J^{12}_0 = J^{21}_0 = 4J = zJ$. The specific volume per lattice point on the underlying fcc lattice is $V/N = \frac{1}{4}a^3$. Then T_c will be evaluated using Eq. (24), with the continuum limit, as

$$I = \frac{1}{4} \int_{\mathrm{BZ}} \frac{d^3q}{(2\pi)^3} \left\{1 - \frac{1}{4}\left[1 + \cos\frac{q_x}{2}\cos\frac{q_y}{2} + \cos\frac{q_y}{2}\cos\frac{q_z}{2} + \cos\frac{q_z}{2}\cos\frac{q_x}{2}\right]\right\}^{-1}. \tag{39}$$

The BZ for the fcc lattice is a bcc Wigner-Seitz cell, with lattice constant $4\pi/a$. We can change the integration region to the cube, $-2\pi \leqslant q_x \leqslant 2\pi, -2\pi \leqslant q_y \leqslant 2\pi, -2\pi \leqslant q_z \leqslant 2\pi$, which contains two copies of the BZ, and include a factor of $\frac{1}{2}$. We also make the variable change, $\mathbf{q}/2 \rightarrow \mathbf{q}$, which gives a factor of 2^3, to get

$$I = 4\frac{1}{(2\pi)^3} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} dq_x dq_y dq_z \{3 - \cos q_x \cos q_y - \cos q_y \cos q_z - \cos q_z \cos q_x\}^{-1}. \tag{40}$$

The integral was also evaluated by Watson[15] to be $I = 4 \times 0.448\,220\,4\ldots = 1.792\,88\ldots$. Thus the critical temperature is estimated as

$$k_B T_c = \frac{4JS^2}{n} \frac{1}{1.792\,88} = \frac{2.231\,05}{n} JS^2. \tag{41}$$

The exact result for T_c (Ising model, $n = 1$) as estimated from series expansions, is known to be $k_B T_c = 2.7040 JS^2$. Thus the ORF calculation, as is usual, underestimates T_c but is a considerable improvement over the simple mean-field result, $k_B T_c = 4JS^2$.

VI. SIMPLE HEXAGONAL BRAVAIS LATTICES AND HCP LATTICES

Another example of a lattice with a basis is the hcp system, which can be considered as interpenetrating simple hexagonal Bravais lattices[14] (i.e., stacked triangular nets). The primitive vectors of the simple hexagonal Bravais lattice can be taken as $\mathbf{a}_1=a\hat{x}, \mathbf{a}_2=a[\frac{1}{2}\hat{x}+(\sqrt{3}/2)\hat{y}], \mathbf{a}_3=c\hat{z}$, where a and c are the lattice constants. For the hcp system, a two-atom basis of $\{\mathbf{0},\mathbf{d}\}$ is used, where $\mathbf{d}=\frac{1}{3}(\mathbf{a}_1+\mathbf{a}_2)+\frac{1}{2}\mathbf{a}_3$, and one triangular net is stacked on top of the previous one, but shifted to be over the centers of one set of the triangular cells below, in what is usually referred to as the $ABAB\ldots$ packing. For the lattice constant ratio $c/a=\sqrt{8/3}$, the highest density packing is obtained, however, for the calculation here this ratio does not directly enter, and need not be specified. Instead, it is interesting to consider that the near-neighbor exchange interactions within the triangular nets (xy plane) have one strength, J_{xy}, while there is a different strength, J_z, for the bonds between the planes. In general we can consider the calculation of T_c as a function of the ratio, $\Delta \equiv J_z/J_{xy}$.

We present first the calculation of $T_c(\Delta)$ for the simple hexagonal Bravais lattice, using the standard ORF theory, which acts as an introduction to the corresponding calculation for the hcp system, because they both rely on the same information concerning the Brillouin zone.

A. Simple hexagonal Bravais lattice

Here there are six neighbor displacements from some arbitrary site to neighbors in the same plane $\{\pm\mathbf{a}_1, \pm\mathbf{a}_2, \pm(\mathbf{a}_1-\mathbf{a}_2)\}$, with exchange strength J_{xy}. The remaining two neighbors, with displacements, $\pm\mathbf{a}_3$, have exchange strengths J_z. A short calculation shows that the q-space exchange [Eq. (10)] is

$$J_{\mathbf{q}}=2J_{xy}[\cos\mathbf{q}\cdot\mathbf{a}_1+\cos\mathbf{q}\cdot\mathbf{a}_2+\cos\mathbf{q}\cdot(\mathbf{a}_1-\mathbf{a}_2)]+2J_z\cos\mathbf{q}\cdot\mathbf{a}_3 \tag{42a}$$

$$=2J_{xy}\left[\cos q_x a+2\cos\frac{1}{2}q_x a\cos\frac{\sqrt{3}}{2}q_y a\right]+2J_z\cos q_z c, \tag{42b}$$

and $J_{\mathbf{0}}=6J_{xy}+2J_z=2(3+\Delta)J_{xy}$ will determine the mean-field critical temperature.

The area of one triangle in the net is $\frac{1}{2}a\times(\sqrt{3}/2)a=(\sqrt{3}/4)a^2$, and there is $\frac{1}{2}$ site per triangle per layer. Thus the specific volume per site is $V/N=(\sqrt{3}/2)a^2c$. The primitive vectors of the reciprocal space are

$$\mathbf{b}_1=\frac{4\pi}{\sqrt{3}a}\left(\frac{\sqrt{3}}{2}\hat{x}-\frac{1}{2}\hat{y}\right), \tag{43a}$$

$$\mathbf{b}_2=\frac{4\pi}{\sqrt{3}a}\hat{y}, \tag{43b}$$

$$\mathbf{b}_3=\frac{2\pi}{c}\hat{z}. \tag{43c}$$

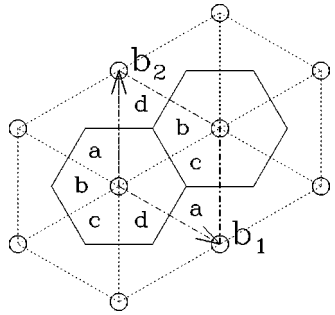

FIG. 1. Wigner-Seitz cells (solid line hexagons) for the simple hexagonal Bravais lattice reciprocal space, compared with the equivalent rhombic cell (dot dash) used for integrals. Segments labeled *a,b,c,d* are equivalent by symmetry operations.

The reciprocal space is another simple hexagonal lattice, with lattice constants $4\pi/\sqrt{3}a$ in the xy plane and $2\pi/c$ in the z direction, rotated by 30° from the real-space lattice. The Brillouin zone Wigner-Seitz cell is a hexagonal cylinder, however, for the purpose of the integral needed here [Eq. (27)] it is more convenient to do the summation inside a cell bounded in the xy plane by a rhombus formed by $\mathbf{b}_1$ and $\mathbf{b}_2$ (see Fig. 1). The hexagonal cylinder and rhombical cylinder cells have equal areas and are equivalent to each other by appropriate symmetry operations. This rhombical cylinder cell is very convenient for evaluation of the integral I, especially with the variable change on $\mathbf{q}$:

$$\mathbf{q}=x\mathbf{b}_1+y\mathbf{b}_2+z\mathbf{b}_3, \tag{44}$$

where the dimensionless parameters x,y,z all range from 0 to 1, mapping out the entire cell. This leads to

$$d^3q=\mathbf{b}_1\cdot(\mathbf{b}_2\times\mathbf{b}_3)dxdydz=(2\pi)^3\frac{N}{V}dxdydz, \tag{45}$$

and the integral is simplified to

$$I=\int_0^1 dx\int_0^1 dy\int_0^1 dz\left\{1-\frac{1}{3+\Delta}[\cos 2\pi x+\cos 2\pi y+\cos 2\pi(x-y)+\Delta\cos 2\pi z]\right\}^{-1}. \tag{46}$$

The integral gives the correction to the mean-field prediction, i.e.,

$$k_BT_c=\frac{k_BT_c^{MF}}{I},\quad k_BT_c^{MF}=\frac{2(3+\Delta)J_{xy}S^2}{n}. \tag{47}$$

The integral I was evaluated numerically by sampling x,y,z uniformly on a cubic grid, with a constant increment $1/N_x$, and then using an extrapolation of the results in the limit that the increment goes to zero. A plot of I versus $1/N_x$ results in a straight line whose extrapolation to $1/N_x\to 0$ gives a very accurate estimate of the integral. (Errors in the integral estimate clearly go as $1/N_x$.) Results obtained for a range of anisotropy parameter $0<\Delta\leqslant 2$ are shown in Fig. 2. At the isotropic limit, $\Delta=1$, we get $I=1.449\,30$ and $nk_BT_c=5.5199JS^2$. In the limit $\Delta\to 0$, the system becomes two dimensional, the integral I diverges logarithmically due to small-$\mathbf{q}$ contributions, and ORF is not applicable.

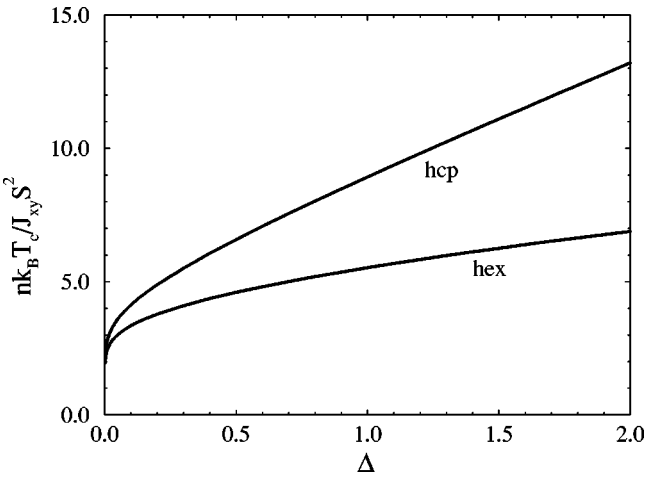

FIG. 2. ORF results for T_c on the simple hexagonal Bravais lattice (hex) and the hexagonal close-packed lattice (hcp), as functions of the exchange anisotropy $\Delta = J_z/J_{xy}$.

B. Hexagonal close-packed lattices

Again there are six neighbor displacements from an arbitrary site to neighbors in the same plane $\{\pm\mathbf{a}_1, \pm\mathbf{a}_2, \pm(\mathbf{a}_1 - \mathbf{a}_2)\}$, with exchange strength J_{xy}. The difference from the simple hexagonal lattice is that there are three neighbors in a layer above and three neighbors in a layer below the one being considered, with exchange couplings J_z, giving 12 neighbors in all. However, to evaluate the matrix elements $J^{i,j}_{\mathbf{r}}$, we need to consider these couplings from the point of view of the simple hexagonal Bravais lattice with a basis (see Fig. 3). The two sites for a given Bravais lattice point can be considered as belonging to two sublattices, 1 and 2. An arbitrary 1 site has the six neighbor displacements to other 1 sites in the same xy plane: $\{\pm\mathbf{a}_1, \pm\mathbf{a}_2, \pm(\mathbf{a}_1 - \mathbf{a}_2)\}$. which will give nonzero J^{11} coupling terms. The neighbors in adjacent planes are 2 sites, leading to nonzero J^{12} terms. Further consideration leads to the nonzero coupling elements,

$$J^{11}_{\mathbf{r}} = J^{22}_{\mathbf{r}} = J_{xy}, \mathbf{r} = \{\pm\mathbf{a}_1, \pm\mathbf{a}_2, \pm(\mathbf{a}_1 - \mathbf{a}_2)\}, \quad (48a)$$

$$J^{12}_{-\mathbf{r}} = J^{21}_{\mathbf{r}} = J_z, \mathbf{r} = \{\mathbf{0}, \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_3 + \mathbf{a}_1, \mathbf{a}_3 + \mathbf{a}_2\}. \quad (48b)$$

It is notable that it is the first example where the diagonal elements are nonzero. The terms where $\mathbf{r} = \mathbf{0}$ are the coupling within the basis.

The q space couplings [Eq. (10)] are found to be

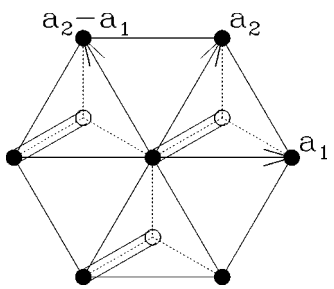

FIG. 3. XY projection of some nearest-neighbor bonds between 1 sites (solid circles) and 2 sites (open circles) in an hcp lattice. Double solid lines connect 1, 2 sites at the same Bravais lattice point. Solid lines show 1-1 bonds (within the planes), dotted lines show 1-2 bonds.

$$J^{11}_{\mathbf{q}} = J^{22}_{\mathbf{q}} = 2J_{xy}[\cos\mathbf{q}\cdot\mathbf{a}_1 + \cos\mathbf{q}\cdot\mathbf{a}_2 + \cos\mathbf{q}\cdot(\mathbf{a}_1 - \mathbf{a}_2)], \quad (49)$$

$$J^{12}_{\mathbf{q}} = (J^{21}_{\mathbf{q}})^* = J_z[1 + e^{-i\mathbf{q}\cdot\mathbf{a}_1} + e^{-i\mathbf{q}\cdot\mathbf{a}_2} + e^{-i\mathbf{q}\cdot\mathbf{a}_3} + e^{-i\mathbf{q}\cdot(\mathbf{a}_3+\mathbf{a}_1)} + e^{-i\mathbf{q}\cdot(\mathbf{a}_3+\mathbf{a}_2)}], \quad (50)$$

and what is needed for evaluation of T_c:

$$J^{12}_{\mathbf{q}} J^{21}_{\mathbf{q}} = J_z^2\{6 + 4[\cos\mathbf{q}\cdot\mathbf{a}_1 + \cos\mathbf{q}\cdot\mathbf{a}_2 + \cos\mathbf{q}\cdot(\mathbf{a}_1 - \mathbf{a}_2)]\} \times [1 + \cos\mathbf{q}\cdot\mathbf{a}_3]. \quad (51)$$

The $q = 0$ exchange strength [Eq. (25)] is seen to be $J_0 = 6(J_{xy} + J_z) = 6J_{xy}(1 + \Delta)$ and determines the Δ-dependent mean-field critical temperature. The specific volume per site (for the underlying simple hexagonal Bravais lattice) is $V/N = (\sqrt{3}/2)a^2c$. The reciprocal space is that of the simple hexagonal Bravais lattice as described in Sec. VI A. Therefore using the rhombical cylinder Brillouin zone cell, the sum I of Eq. (24) is transformed into an integral using Eqs. (44) and (45) over a cubic region,

$$\frac{1}{N}\sum_{\mathbf{q}} \rightarrow \int_0^1 dx \int_0^1 dy \int_0^1 dz. \quad (52)$$

The integrand depends on the transformed quantities

$$J^{11}_{\mathbf{q}} = 2J_{xy}[\cos 2\pi x + \cos 2\pi y + \cos 2\pi(x - y)], \quad (53a)$$

$$J^{12}_{\mathbf{q}} J^{21}_{\mathbf{q}} = 2J_{xy}\Delta[1 + \cos 2\pi z] \times \{3 + 2[\cos 2\pi x + \cos 2\pi y + \cos 2\pi(x - y)]\}. \quad (53b)$$

The correction to the mean-field prediction is

$$k_B T_c = \frac{k_B T_c^{MF}}{I}, \quad k_B T_c^{MF} = \frac{6(1 + \Delta)J_{xy}S^2}{n}. \quad (54)$$

I was evaluated by the numerical techniques described above (Sec. VI A), including the $N_x \rightarrow \infty$ extrapolation. At the isotropic limit, $\Delta = 1$, we get $I = 1.344\,66$, and $nk_BT_c = 8.924\,18JS^2$. It is interesting to note that the same value of I results for the fcc lattice [Eq. (27)], when evaluated to the same precision. Thus the ORF corrections to the mean-field T_c for fcc and hcp lattices, both with 12 nearest neighbors, are the same. Some other hcp results in a limited range of anisotropy Δ are shown in Fig. 2. Once again, in the limit $\Delta \rightarrow 0$ there is a weak divergence of the integral as the system crosses over into a two-dimensional one, with $T_c \rightarrow 0$ over a very narrow range of Δ. ORF is not applicable in this limit; T_c should pass over to the finite value for the 2D triangular lattice model.[19]

There are a few theoretical results to compare with for the hcp system. In a series of papers, Domany, Gubernatis, and Auerbach[20–22] analyzed a Lifshitz tricritical point for the hcp Ising model, which occurs at a negative value of Δ. As part of their analysis they applied Monte Carlo calculations[21] to determine the phase diagram; very roughly for $\Delta = 1$ they obtained $k_BT_c \approx 10JS^2$. Values of T_c at other anisotropies also can be estimated from their Fig. 1 but with poor precision. Monte Carlo simulations by Hashibon *et al.*[12] demon-

strated $k_B T_c \approx 10JS^2$ with greater precision for the isotropic hcp Ising system. Therefore it does appear that the Onsager results fall below the Monte Carlo estimates of T_c, as expected.

For the hcp Heisenberg model, Adler[23] estimated T_c by a Green's-function approach together with a random-phase approximation. It is surprising to see that at $\Delta=1$ Alder found the correction to the mean-field T_c to be by a factor $F(-1)=1.34\pm0.005$, where $F(-1)$ is a certain sum over the Brillouin zone. Making a more accurate evaluation by the techniques described here, we get $F(-1)=1.344\,66$, i.e., a value exactly equal to the correction integral I obtained from the ORF procedure. In order to compare carefully to the Adler result (for spin 1/2), we should note that a factor of $2S(S+1)$, implicitly included there in the expression for T_c, must be replaced by S^2 here, to cancel the double counting of bonds and to compare quantum and classical results. Then, it is easy to show that the expression for $F(-1)$ given by Adler is exactly equivalent to our expression (26) for I, including the anisotropic case, $\Delta\neq1$, Therefore the Green's-function approach used there is exactly equivalent to the ORF procedure presented here; they are different approaches to impose the random-phase approximation.

Furthermore, in this level of approximation, the question posed by Domb and Sykes[24] and investigated by Adler is answered: T_c for fcc and hcp Ising models are the same, even though the hcp lattice is more densely packed and might be expected to have a higher T_c. Apparently a more precise procedure is needed to determine whether there is a true difference in their critical temperatures.

VII. REACTION FIELD AND THERMODYNAMIC QUANTITIES AT $T>T_C$

It is clear that any quantities such as specific heat, magnetization, etc., can be evaluated via the RPA Hamiltonian for temperatures away from T_c, provided that the reaction field λ has been determined. Thus we take a few sentences to examine how λ can be calculated.

At the critical temperature, the reaction field as determined from Eq. (23) is seen to be

$$\lambda_c \equiv \lambda(T_c) = \frac{1}{2}(J_0 - \chi_0^{-1}) = \frac{1}{2}(J_0 - nk_B T_c/S^2). \quad (55)$$

For higher temperatures, the constraining Eq. (22) to determine λ is equivalent to

$$\frac{V}{N}\int_{BZ}\frac{d^3q}{(2\pi)^3}\,\frac{1-\chi_0(J_{\mathbf{q}}^{11}-2\lambda)}{[1-\chi_0(J_{\mathbf{q}}^{11}-2\lambda)]^2-\chi_0^2 J_{\mathbf{q}}^{12}J_{\mathbf{q}}^{21}} = 1. \quad (56)$$

Considering the left-hand side as a function of λ, one can apply Newton's method to search for the λ at which the function passes through 1. This search can be aided by the requirement that the denominator of this integrand must be positive everywhere in the BZ, including at $\mathbf{q}=0$. This leads to the inequality for $T>T_c$,

$$\frac{1}{2}(J_0 - nk_B T/S^2) < \lambda(T) < \lambda_c. \quad (57)$$

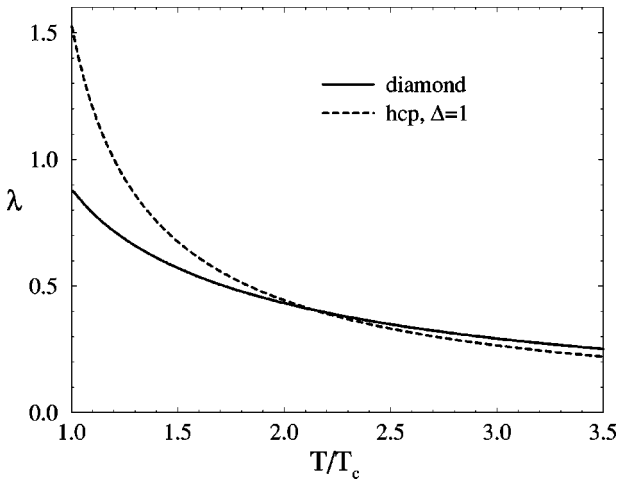

FIG. 4. The reaction field λ for $T>T_c$ for the diamond lattice and isotropic hexagonal close-packed lattice ($\Delta=1$).

Results for $\lambda(T)$ for the diamond lattice and hcp lattice (at $\Delta=1$) are shown in Fig. 4. As a function of T/T_c, λ does not depend on the number of spin components n. The hcp lattice, which has higher coordination number, also has the stronger reaction field at T_c. As the temperature is increased, the reaction fields diminish and become of comparable sizes for $T>2T_c$. It is also expected that the slope relates to the specific heat.[7] The graph then reasonably demonstrates a larger specific heat for hcp compared to diamond near T_c, in contrast to more similar specific heats at higher temperatures.

VIII. CONCLUSIONS

We have reviewed the standard Onsager reaction field approximation for estimating T_c, and have shown how it can be extended to apply to a Bravais lattice with a basis. The bcc lattice was used as a test case because it can be calculated either by the standard approach or our method, when considered as sc with a two-atom basis. We used our method to get T_c for diamond and anisotropic hcp lattice systems, however, it certainly can be extended to more complex systems with a greater number of atoms per unit cell. For the hcp lattice system, the ORF procedure used here was found to be exactly equivalent to a Green's function (plus RPA) approach used by Adler.[23] This equivalence of the Green-function[17,18] and ORF approaches also is known to hold for the sc, bcc, and fcc lattices. While it is an approximate method, ORF is very physically motivated, and does give reasonable estimates of T_c and other quantities where other methods may be more cumbersome or time consuming to apply.

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