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The critical temperature of a fully anisotropic three-dimensional Ising model

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Abstract. The critical temperature of a three-dimensional Ising model on a simple cubic lattice with different coupling strengths along all three spatial directions is calculated via the transfer matrix method and a finite-size scaling for $L \times L \times \infty$ clusters ($L = 2$ and 3). The results obtained are compared with available calculations. An exact analytical solution is found for the $2 \times 2 \times \infty$ Ising chain with fully anisotropic interactions (arbitrary J_x, J_y and J_z).

1. Introduction

Great attention has been given to the critical temperature calculation of the three-dimensional Ising model, for the full time extent of its existence. The most considerable advances have been attained for the fully isotropic cubic lattice ($J_x = J_y = J_z$). The calculations are steadily improving with time; the accuracy for the critical point value is down to $10^{-3}\%$ error: $K_c = 0.221\,659\,5 \pm 0.000\,002\,6$ (Ferrenberg and Landau 1991); $K_c = 0.221\,654\,4 \pm 0.000\,001\,0$ (Livet 1991).

The efficiency of progress is less for the partly anisotropic model when $J_x = J_y \neq J_z$. Two cases exist here: $J_x = J_y \geqslant J_z$ (a quasi-two-dimensional model) and, inversely, $J_x = J_y \leqslant J_z$ (a quasi-one-dimensional model). Using the high-temperature series, the critical temperature estimates have been obtained with $2 \times 10^{-2}\%$ error for the fully isotropic interactions ($J_x = J_y = J_z$) and about $10^{-3}\%$ in the two-dimensional limit ($J_z = 0$) of the quasi-two-dimensional model (see Navarro and de Jongh (1978) and references therein). By intermediate-range interlayer couplings, the error of a phase transition temperature determination lies between these two extreme values. Conversely, in the quasi-one-dimensional case, the estimates based on the same high-temperature series rapidly deteriorate owing to the limited number of terms available in the series. As a result, one can find the critical temperatures only up to $J_{x(y)}/J_z = 10^{-2}$ (with exactness in the one- to two-significant-figure range). In the quasi-one-dimensional case, the phase transition temperature has been calculated also by phenomenological renormalization of clusters (Yurishchev and Sterlin 1991). Inasmuch as the cluster geometry reflects the physical situation, this approach (contrary to the high-temperature series expansions) yields more precise results as the anisotropy of the quasi-one-dimensional system increases. By $J_{x(y)}/J_z = 10^{-3}$, the critical-temperature position is determined here with an accuracy of about three significant figures.

The difficulties are largest when the interactions are different along all three directions. Here calculations have been done by the real-space renormalization group method (da Silva *et al* 1984) and via various versions of the mean-field theory and variational principle (see Faleiro Ferreira (1988, 1989) and references therein). These results we discuss in detail in section 3 in comparison with our computations.

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In this paper, the critical temperature of a three-dimensional Ising model, with fully anisotropic interactions, is calculated by the transfer matrix approach in combination with a finite-size scaling, i.e. by the phenomenological renormalization group method proposed by Nightingale (1976). As the clusters, we use infinitely long parallelepipeds $L \times L \times \infty$ with transverse scales $L = 2$ and 3. We succeeded in obtaining a rigorous solution for a lattice with $L = 2$. For the $3 \times 3 \times \infty$ lattice, we simplify the partial eigenvalue problem for the transfer matrix of 512th order. Using the symmetry, we reduce this problem to a determination of the largest eigenvalues of the two eighteenth-order matrices. Final calculations have already been made numerically.

2. Calculation of the critical temperature

Conforming with the phenomenological renormalization group theory, the critical temperature T_c is a fixed point of an equation (see, for instance, the reviews of Nightingale (1982) and Barber (1983)):

$$L\kappa_L(T_c) = L'\kappa_{L'}(T_c) \tag{1}$$

where

$$\kappa_L = \ln(\lambda_1/\lambda_2) \tag{2}$$

is the inverse correlation length in a cluster with characteristic size L. The quantities λ_1 and λ_2 entering into (2) are the largest and next-largest eigenvalues, respectively, of the subsystem transfer matrix. Thus, the task is reduced to finding the dominant eigenvalues of transfer matrices.

2.1. *Cluster* $2 \times 2 \times \infty$

Let us write the Hamiltonian for the cluster as

$$H = -\sum_i [J_x(\sigma_{1,i}\sigma_{2,i} + \sigma_{3,i}\sigma_{4,i}) + J_y(\sigma_{1,i}\sigma_{4,i} + \sigma_{2,i}\sigma_{3,i}) + J_z(\sigma_{1,i}\sigma_{1,i+1} + \sigma_{2,i}\sigma_{2,i+1} + \sigma_{3,i}\sigma_{3,i+1} + \sigma_{4,i}\sigma_{4,i+1})]. \tag{3}$$

The spin variables $\sigma = \pm 1$ are located in sites of a lattice $2 \times 2 \times \infty$ which has a rectangular cross section and has the symmetry planes going through its axis and the middles of opposite sides.

The transfer matrix $\mathbf{U}$ with elements

$$\langle \sigma_1, \sigma_2, \sigma_3, \sigma_4 | \mathbf{U} | \sigma_1', \sigma_2', \sigma_3', \sigma_4' \rangle = \exp[\tfrac{1}{2}K_x(\sigma_1\sigma_2 + \sigma_3\sigma_4 + \sigma_1'\sigma_2' + \sigma_3'\sigma_4') + \tfrac{1}{2}K_y(\sigma_1\sigma_4 + \sigma_2\sigma_3 + \sigma_1'\sigma_4' + \sigma_2'\sigma_3') + K_z(\sigma_1\sigma_1' + \sigma_2\sigma_2' + \sigma_3\sigma_3' + \sigma_4\sigma_4')] \tag{4}$$

(where $K_x = J_x/kT$, $K_y = J_y/kT$ and $K_z = J_z/kT$) corresponds to the Hamiltonian (3).

To solve the eigenvalue problem of the transfer matrix (4), we use first the invariance property of the appropriate Hamiltonian with respect to the transformations of the group $Z_2 \otimes C_{2v}$; where Z_2 is a group of global reflections in the spin space, C_{2v} is the point group generated by the symmetry planes of a lattice and $\otimes$ represents the direct product. Carrying out the usual group-theoretical analysis (see, e.g., Yurishchev (1989)), we come

to a conclusion that the 16×16 transfer matrix (4) can be reduced owing to symmetry $Z_2 \otimes C_{2v}$ to a quasi-diagonal form with one subblock 5×5, four subblocks 2×2 and three 'subblocks' 1×1, i.e. ready-made eigenvalues.

The subblock of size 5×5 is connected with the fully symmetrical irreducible representation of the group. Because of the Perron theorem, it contains the largest eigenvalue of $\mathbf{U}$. The basis vectors for this irreducible representation are given as

$$\begin{aligned} &\psi_1 = (e_1 + e_{16})/\sqrt{2} \qquad \psi_2 = (e_2 + e_3 + e_5 + e_8 + e_9 + e_{12} + e_{14} + e_{15})/2\sqrt{2} \\ &\psi_3 = (e_4 + e_{13})/\sqrt{2} \qquad \psi_4 = (e_6 + e_{11})/\sqrt{2} \qquad \psi_5 = (e_7 + e_{10})/\sqrt{2} \end{aligned} \tag{5}$$

where

$$e_1 = |1, 1, 1, 1\rangle \qquad e_2 = |1, 1, 1, -1\rangle \qquad \ldots \qquad e_{16} = |-1, -1, -1, -1). \tag{6}$$

Using these basis functions and utilizing (4), we find the matrix elements $\psi_i^+ \mathbf{U} \psi_j$ of subblock 5×5. The secular equation of this subblock has a structure (and this is the second key circumstance allowing the solution of the eigenvalue problem)

$$\lambda^5 - a_1\lambda^4 + a_2\lambda^3 - \alpha a_2\lambda^2 + \alpha^3 a_1\lambda - \alpha^5 = 0. \tag{7}$$

Here

$$a_1 = 2[1 + 4\cosh(2K_x)\cosh(2K_y)]\cosh(4K_z) + 6 \tag{8}$$

$$\begin{aligned} a_2 = {} & 32\cosh(2K_x)\cosh(2K_y)[\cosh(4K_z)\cosh^2(2K_z) - 1] \\ & + 8[1 + \cosh(4K_x) + \cosh(4K_y)]\sinh^2(4K_z) \end{aligned} \tag{9}$$

$$\alpha = 4\sinh^2(2K_z). \tag{10}$$

According to Sominskii (1967), an algebraic equation such as (7) is a reciprocal equation. This property makes it possible to find the roots of our equation easily. As a result, the largest eigenvalue of the transfer matrix (4) is equal to

$$\lambda_1 = \tfrac{1}{2}r_1 + (\tfrac{1}{4}r_1^2 - \alpha^2)^{1/2} \tag{11}$$

with

$$r_1 = \tfrac{1}{2}(a_1 - \alpha) + [\tfrac{1}{4}(a_1 + \alpha)^2 + \alpha^2 - a_2]^{1/2}. \tag{12}$$

Solving secular equations of second-order subblocks causes no difficulties. In this issue, we obtain a complete set of eigenvalues. Sorting the eigenvalues, we seek out the next largest eigenvalue of $\mathbf{U}$:

$$\begin{aligned} \lambda_2 = {} & \{1 + \exp[2(K_x + K_y)]\}\sinh(4K_z) + [[\{1 - \exp[2(K_x + K_y)]\}^2\sinh^2(4K_z) \\ & + 16\exp[2(K_x + K_y)]\sinh^2(2K_z)]]^{1/2}. \end{aligned} \tag{13}$$

Note that it lies in the subblock built on basis functions which are symmetrical under all purely spatial transformations of the group and antisymmetrical under those including the spin inversion.

By $J_x = J_y$, our solution is reduced to that of Kaufman (1949) for the Ising model on a cylinder, if the number of chains in the last model is equal to four.

It is also interesting to note that the above does not succeed in generalizing the model (3). All attempts to include in the Hamiltonian new interactions (e.g., external field, additional pair couplings or multiparticle forces) lead immutably to the destruction of the obvious symmetry of $Z_2 \otimes C_{2v}$ or the hidden algebraic symmetry (i.e. the reciprocal property of a secular equation).

2.2. Cluster 3 × 3 × ∞

We shall consider a subsystem $3 \times 3 \times \infty$ with cyclic boundary conditions in both transverse directions. This eliminates undesirable surface effects and at the same time extends the symmetry group down to $Z_2 \otimes (T \circledS C_{2v})$, where T is a group of transverse translations and Ⓢ implies a semidirect multiplication. The given symmetry allows one to reduce the transfer matrix **V**, of size 512×512, to a block diagonal form in which the first- and second-largest eigenvalues of the original matrix are located in different subblocks ($\mathbf{V}^{(1)}$ and $\mathbf{V}^{(2)}$, respectively), both having a dimension of 18×18. The open form of these subblocks is given in the appendix. The extraction of dominant eigenvalues from $\mathbf{V}^{(1)}$ and $\mathbf{V}^{(2)}$ has already been carried out by computer.

We return again to the calculation of the critical temperature. The estimates kT_c/J_z obtained by a numerical solution of transcendental equation (1) are collected in table 1. By this, we also put the cyclic boundary conditions on the cluster $2 \times 2 \times \infty$, i.e. simply increase the interaction constants in transverse directions by a factor of 2: $J_x \to 2J_x$ and $J_y \to 2J_y$. In table 1, we have also inserted the critical temperature values for two limited cases:

(i) $J_y = 0$, corresponding to the anisotropic two-dimensional Ising model for which the exact phase transition temperature equation is known (Onsager 1944)

$$\sinh(2J_x/kT_c)\sinh(2J_z/kT_c) = 1 \tag{14}$$

(ii) $J_x = J_y$, corresponding to the partly anisotropic three-dimensional Ising model for which there exists sufficiently accurate estimates of T_c (Navarro and de Jongh 1978, Yurishchev and Sterlin 1991).

3. Discussion

One of the simplest ways to estimate the phase transition temperature in an Ising model is the mean-field approximation (MFA):

$$(kT_c)_{MFA} = 2(J_x + J_y + J_z). \tag{15}$$

However, the accuracy is quite low (see table 2 where, for convenience of comparison, the critical-temperature estimates found by various approximate methods have been given, as well as the true values obtained from a solution of equation (14) and the precision numerical values).

The state of things is somewhat corrected by an improved mean-field approximation (IMFA), taking into account the short-range order effects (Faleiro Ferreira 1988). On inspection of table 2, one can see that there are considerable errors, especially for the strongly anisotropic systems.

The MFA can be considerably improved by placing the clusters in the mean field instead of separate spins. A linear chain approximation (LCA) considered by Stout and Chisholm (1962) when the one-dimensional Ising system is taken as a cluster leads to the equation

$$(kT_c/J_z)_{LCA} = 2\eta \exp(2J_z/kT_c) \tag{16}$$

where $\eta = (J_x + J_y)/J_z$. de Bruijn (1958) has shown that the solution of an equation such as (16) is given by

$$(kT_c/J_z)_{asympt} = 2/\{\ln \eta^{-1} - \ln(\ln \eta^{-1}) + O[\ln(\ln \eta^{-1})/\ln \eta^{-1}]\} \tag{17}$$

Table 1. Normalized critical temperature kT_c/J_z for the fully anisotropic three-dimensional Ising model as a function of J_x/J_z and J_y/J_x.

	J_y/J_x							
	0.0					1.0		
J_x/J_z		Onsager (1944)	0.25	0.50	0.75		Navarro and de Jongh (1978)	Yurishchev and Sterlin (1991)
1.0	2.367	2.269	3.277	3.819	4.275	4.685	4.5106	
0.9	2.246	2.153	3.079	3.575	3.993	4.368		
0.8	2.120	2.034	2.876	3.325	3.704	4.045		
0.7	1.987	1.909	2.667	3.070	3.409	3.714		
0.6	1.848	1.779	2.451	2.806	3.105	3.375		
0.5	1.699	1.641	2.226	2.533	2.791	3.024	2.9286	
0.4	1.540	1.492	1.988	2.247	2.464	2.659	2.580	
0.3	1.365	1.328	1.733	1.943	2.117	2.273	2.219	
0.2	1.167	1.141	1.450	1.608	1.738	1.854	1.814	
0.1	0.921	0.905	1.109	1.211	1.293	1.366	1.343	
0.09	0.891	0.877	1.069	1.164	1.241	1.309		
0.08	0.859	0.846	1.026	1.115	1.187	1.251		
0.07	0.826	0.814	0.982	1.064	1.131	1.189		
0.06	0.790	0.779	0.934	1.010	1.070	1.124		
0.05	0.751	0.741	0.882	0.951	1.006	1.054	1.041	
0.04	0.707	0.698	0.825	0.886	0.935	0.978		
0.03	0.657	0.650	0.760	0.813	0.856	0.892		
0.02	0.597	0.590	0.683	0.727	0.761	0.791		
0.01	0.513	0.508	0.579	0.611	0.637	0.658	0.65	
0.009	0.502	0.498	0.565	0.596	0.621	0.641		0.637
0.008	0.491	0.486	0.551	0.581	0.604	0.624		0.619
0.007	0.478	0.474	0.535	0.564	0.586	0.604		0.600
0.006	0.464	0.460	0.518	0.545	0.566	0.583		0.579
0.005	0.449	0.445	0.499	0.524	0.544	0.560		0.556
0.004	0.431	0.428	0.478	0.501	0.519	0.534		0.531
0.003	0.410	0.407	0.453	0.474	0.490	0.503		0.500
0.002	0.383	0.380	0.421	0.439	0.453	0.465		0.462

Table 2. Critical temperature estimates of the fully anisotropic three-dimensional Ising model versus calculational method.

	$J_x/J_z = 1$		$J_x/J_z = 10^{-2}$	
Method	$J_y = 0$	$J_y = J_x$	$J_y = 0$	$J_y = J_x$
MFA	4	6	2.02	2.04
IMFA	3.230	4.933	1.465	1.487
LCA	3.526	5.686	0.590	0.699
ILCA	2.885	4.622	0.588	0.695
ELCA	2.728	4.881	0.543	0.669
Table 1	2.367	4.685	0.513	0.658
Exact	2.2691	4.5115	0.5089	0.65

when $\eta \to 0$. Fisher (1967) established that equation (17) is asymptotically exact for the Ising model. Although it qualitatively describes the logarithmically slow drop in the critical temperature with increase in the coupling anisotropy, unfortunately this asymptotical formula does not provide acceptable precision, even at high anisotropies. For example, by $J_x = J_y = 10^{-2}J_z$ an error of deviation from the high-temperature series estimate equals

21% and the error is 28% for the two-dimensional model ($J_y = 0$) for the same value of anisotropy ($J_x/J_z = 10^{-2}$).

During recent years a number of equations have been obtained for the critical temperature of a fully anisotropic three-dimensional Ising model within the various generalizations of the mean-field theory, as well as a variational approach (one of them—the IMFA—we have mentioned already). Using an extended variational method and taking the sum of linear Ising chains as an auxiliary Hamiltonian, Faleiro Ferreira and Silva (1982) have found an equation for T_c via the so-called extended linear chain approximation (ELCA). The numerical solution of this equation shows that the ELCA perceptibly improves the LCA (see table 2); however, errors are still considerable. For instance, the critical point position for the two-dimensional isotropic case is overstated by 20%.

Another new approach named by Faleiro Ferreira (1989) the improved linear chain approximation (ILCA) is based upon the same auxiliary Hamiltonian but with another variational principle and leads to better results only for the isotropic three-dimensional case (this is observed in table 2).

da Silva *et al* (1984) have reported the calculation of a phase transition temperature for the fully anisotropic three-dimensional Potts lattice, a particular case of which is the Ising model, by the real-space renormalization group treatment. However, owing to the finite size of spin blocks used, their estimates lose accuracy very rapidly with an increase in coupling anisotropy. Already only by $J_x = J_y = 10^{-1}J_z$, it follows the overestimate $kT_c/J_z = 1.4552$ which, even after carrying out the extrapolation on the rather artificial scheme proposed by these workers, falls to $kT_c/J_z = 1.3986$. This value surpasses the high-temperature series value by 4.1%.

We now consider our results. The application of clusters makes it possible to take into account the specific features of short-range order and, as a result, reduce the calculational error. Therefore, it is not surprising that the finite-size scaling method with its hierarchy of clusters increasing in growth allows us to determine the critical point of the Ising model with more exactness than the approaches discussed above (see again table 2). A uniform convergence (contrary to the ILCA) of the estimates with increase in lattice anisotropy is an important quality of the approximation. Let us consider table 1. In the two-dimensional isotropic limit ($J_y = 0$ and $J_x/J_z = 1$), our calculation fixes the critical temperature with an error of 4.3% (in the direction of overestimation). For $J_x/J_z \to 0$, this error decreases continuously. This can be easily checked by making a comparison with the exact transition temperature values presented in the next column. In particular, the value has a 1.8% error by $J_x/J_z = 10^{-1}$. A similar situation arises in the three-dimensional case with $J_x = J_y$. Here our estimates are again in excess of the true values; the percentage error drops from the maximum value of 3.8% in the fully isotropic case ($J_x = J_y = J_z$) to, for comparison, 1.7% for the $J_x/J_z = 10^{-1}$ case. An analogous picture seems to be preserved in the intermediate region $0 < J_y/J_x < 1$; by fixing J_x/J_z, the error smoothly moves between the limited values corresponding to $J_y/J_x = 0$ and $J_y/J_x = 1$.

4. Conclusions

In the present paper the more qualitative estimates of critical temperature in the fully anisotropic three-dimensional Ising lattice have been derived. These estimates yield the upper bound everywhere and by $J_y/J_x =$ constant the error for kT_c/J_z monotonically tends to zero when $J_x/J_z \to 0$.

The accurate analytical solution has been obtained for an Ising model on the $2 \times 2 \times \infty$ lattice with fully anisotropic couplings.

The quasi-diagonalization has been carried out for the transfer matrix of the $3 \times 3 \times \infty$ Ising model with a rectangular cross section. The expressions for the matrix elements of subblocks containing the leading eigenvalues are given in detail. This permits one to reproduce easily the results presented in the article; it could also be useful in considering other problems.

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Appendix. Explicit form of subblocks $\mathbf{V}^{(1)}$ and $\mathbf{V}^{(2)}$

The matrices $\mathbf{V}^{(1)}$ and $\mathbf{V}^{(2)}$ are symmetrical; therefore, it is sufficient to describe their upper triangular parts:

$$V_{ij}^{(1)} = 2\sqrt{\frac{n_j}{n_i}}\left(\sum_{s=1}^{5} |g_s^{(i,j)}| \cosh[(2s-1)K_z]\right) \exp[\tfrac{1}{2}(m_i^a + m_j^a)K_x + \tfrac{1}{2}(m_i^b + m_j^b)K_y] \quad \text{(A1)}$$

$$V_{ij}^{(2)} = 2\sqrt{\frac{n_j}{n_i}}\left(\sum_{s=1}^{5} g_s^{(i,j)} \sinh[(2s-1)K_z]\right) \exp[\tfrac{1}{2}(m_i^a + m_j^a)K_x + \tfrac{1}{2}(m_i^b + m_j^b)K_y] \quad \text{(A2)}$$

where $i \leqslant j = 1, 2, \ldots, 18$. The basis vectors are ordered with their lengths not decreasing:

$$n_i = \{2, 6, 6, 12, 18, 18, 18, 18, 18, 36, 36, 36, 36, 36, 36, 36, 72, 72\}. \quad \text{(A3)}$$

The quantities m_i^a and m_i^b are equivalent to the reduced partial energies of spin configurations in the ith vector. They are

$$m_i^a = \{9, 9, -3, -3, 5, 5, 1, 1, -3, 1, 1, -3, 5, -3, 1, -3, 1, -3\} \quad \text{(A4)}$$

$$m_i^b = \{9, -3, 9, -3, 5, 1, 5, 1, -3, 1, -3, 1, -3, 5, -3, 1, 1, -3\}. \quad \text{(A5)}$$

Finally, the weight coefficients $g_s^{(i,j)}$ are given as follows:

1,1) 0 0 0 0 1	1,2) 0 1 0 0 0	2,2) 0 −2 0 0 1	1,3) 0 1 0 0 0
2,3) 3 0 0 0 0	3,3) 0 −2 0 0 1	1,4) 0 1 0 0 0	2,4) 3 0 0 0 0
3,4) 3 0 0 0 0	4,4) 3 −2 0 0 1	1,5) 0 0 0 1 0	2,5) 2 0 1 0 0
3,5) 2 0 1 0 0	4,5) 4 0 2 0 0	5,5) 0 0 8 0 1	1,6) 0 0 1 0 0
2,6) −2 0 0 1 0	3,6) −1 2 0 0 0	4,6) −2 4 0 0 0	5,6) 0 7 0 2 0
6,6) 6 0 2 0 1	1,7) 0 0 1 0 0	2,7) −1 2 0 0 0	3,7) −2 0 0 1 0
4,7) −2 4 0 0 0	5,7) 0 7 0 2 0	6,7) 5 0 4 0 0	7,7) 6 0 2 0 1
1,8) 1 0 0 0 0	2,8) 0 2 −1 0 0	3,8) 0 2 −1 0 0	4,8) −4 2 0 0 0
5,8) −5 4 0 0 0	6,8) 4 −3 2 0 0	7,8) 4 −3 2 0 0	8,8) 4 −4 0 0 1
1,9) 1 0 0 0 0	2,9) −2 1 0 0 0	3,9) −2 1 0 0 0	4,9) 0 4 −2 0 0
5,9) −5 4 0 0 0	6,9) 6 −2 1 0 0	7,9) 6 −2 1 0 0	8,9) 8 0 0 −1 0
9,9) 4 −4 0 0 1	1,10) 0 0 1 0 0	2,10) −1 2 0 0 0	3,10) −1 2 0 0 0
4,10) −3 2 0 1 0	5,10) 0 7 0 2 0	6,10) 5 0 4 0 0	7,10) 5 0 4 0 0
8,10) 6 −2 1 0 0	9,10) 4 −3 2 0 0	10,10) 11 0 6 0 1	1,11) 0 1 0 0 0
2,11) 1 −1 1 0 0	3,11) 3 0 0 0 0	4,11) 2 −2 2 0 0	5,11) 6 0 3 0 0
6,11) −4 4 0 1 0	7,11) −3 6 0 0 0	8,11) −4 4 −1 0 0	9,11) −5 2 −1 1 0
10,11) −8 8 0 2 0	11,11) 9 −5 3 0 1	1,12) 0 1 0 0 0	2,12) 3 0 0 0 0

3,12) 1 −1 1 0 0 4,12) 2 −2 2 0 0 5,12) 6 0 3 0 0 6,12) −3 6 0 0 0
7,12) −4 4 0 1 0 8,12) −4 4 −1 0 0 9,12) −5 2 −1 1 0 10,12) −8 8 0 2 0
11,12) 10 −4 4 0 0 12,12) 9 −5 3 0 1 1,13) 1 0 0 0 0 2,13) −1 0 −1 1 0
3,13) −2 1 0 0 0 4,13) −4 2 0 0 0 5,13) −5 4 0 0 0 6,13) 2 −4 3 0 0
7,13) 6 −2 1 0 0 8,13) 4 −2 2 −1 0 9,13) 5 −3 1 0 0 10,13) 12 −4 2 0 0
11,13) −7 7 −3 1 0 12,13) −12 6 0 0 0 13,13) 3 −7 5 −2 1 1,14) 1 0 0 0 0
2,14) −2 1 0 0 0 3,14) −1 0 −1 1 0 4,14) −4 2 0 0 0 5,14) −5 4 0 0 0
6,14) 6 −2 1 0 0 7,14) 2 −4 3 0 0 8,14) 4 −2 2 −1 0 9,14) 5 −3 1 0 0
10,14) 12 −4 2 0 0 11,14) −12 6 0 0 0 12,14) −7 7 −3 1 0 13,14) 10 −6 2 0 0
14,14) 3 −7 5 −2 1 1,15) 1 0 0 0 0 2,15) 0 2 −1 0 0 3,15) −2 1 0 0 0
4,15) −2 3 −1 0 0 5,15) −5 4 0 0 0 6,15) 4 −3 2 0 0 7,15) 6 −2 1 0 0
8,15) 3 −4 2 0 0 9,15) 3 −4 2 0 0 10,15) 10 −5 3 0 0 11,15) −10 4 −2 2 0
12,15) −8 8 −2 0 0 13,15) 8 −4 4 −2 0 14,15) 10 −6 2 0 0 15,15) 7 −8 2 0 1
1,16) 1 0 0 0 0 2,16) −2 1 0 0 0 3,16) 0 2 −1 0 0 4,16) −2 3 −1 0 0
5,16) −5 4 0 0 0 6,16) 6 −2 1 0 0 7,16) 4 −3 2 0 0 8,16) 3 −4 2 0 0
9,16) 3 −4 2 0 0 10,16) 10 −5 3 0 0 11,16) −8 8 −2 0 0 12,16) −10 4 −2 2 0
13,16) 10 −6 2 0 0 14,16) 8 −4 4 −2 0 15,16) 11 −4 2 −1 0 16,16) 7 −8 2 0 1
1,17) 0 1 0 0 0 2,17) 1 −1 1 0 0 3,17) 1 −1 1 0 0 4,17) 4 −1 1 0 0
5,17) 6 0 3 0 0 6,17) −4 4 0 1 0 7,17) −4 4 0 1 0 8,17) −5 2 −1 1 0
9,17) −4 4 −1 0 0 10,17) −7 10 0 1 0 11,17) 10 −4 4 0 0 12,17) 10 −4 4 0 0
13,17) −7 7 −3 1 0 14,17) −7 7 −3 1 0 15,17) −9 6 −2 1 0 16,17) −9 6 −2 1 0
17,17) 19 −9 7 0 1 1,18) 1 0 0 0 0 2,18) −2 1 0 0 0 3,18) −2 1 0 0 0
4,18) −3 1 −1 1 0 5,18) −5 4 0 0 0 6,18) 6 −2 1 0 0 7,18) 6 −2 1 0 0
8,18) 5 −3 1 0 0 9,18) 4 −2 2 −1 0 10,18) 8 −6 4 0 0 11,18) −7 7 −3 1 0
12,18) −7 7 −3 1 0 13,18) 10 −6 2 0 0 14,18) 10 −6 2 0 0 15,18) 9 −5 3 −1 0
16,18) 9 −5 3 −1 0 17,18) −19 13 −3 1 0 18,18) 13 −13 7 −2 1.

Using (A1)–(A5) and the above values for the weight coefficients, one can easily find the expressions for the matrix elements. For instance,

$$V_{11}^{(1)} = 2\cosh(9K_z)\exp[9(K_x + K_y)]$$

$$V_{35}^{(1)} = 2\sqrt{3}[2\cosh(K_z) + \cosh(5K_z)]\exp(K_x + 7K_y)$$

$$V_{18,18}^{(2)} = 2\{13[\sinh(K_z) - \sinh(3K_z)] + 7\sinh(5K_z) - 2\sinh(7K_z) + \sinh(9K_z)\} \times \exp[-3(K_x + K_y)].$$

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