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# Curie and Néel temperatures of quantum magnets

**J Oitmaa and Weihong Zheng**

School of Physics, The University of New South Wales, Sydney, NSW 2052, Australia

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**Abstract**
We estimate, using high-temperature series expansions, the transition temperatures of the spin $\frac{1}{2}$, 1 and $\frac{3}{2}$ Heisenberg ferromagnet and antiferromagnet in three dimensions. The manner in which the difference between Curie and Néel temperatures vanishes with increasing spin quantum number is investigated.

It is well known that in classical spin models, such as the Ising and classical Heisenberg models, on bipartite lattices the critical temperature (if it exists) is the same for ferromagnetic exchange (Curie temperature) as for antiferromagnetic exchange (Néel temperature). This is a direct consequence of the free energy being an even function of the exchange parameter $J$. It has also been known for some time, but perhaps less widely, that for the quantum spin $\frac{1}{2}$ Heisenberg model the Curie and Néel temperatures are unequal. Early work [1, 2] put the Néel temperature some 10% above the Curie temperature for spin $\frac{1}{2}$, for both the simple cubic (SC) and body centred cubic (BCC) lattices, with the difference decreasing rapidly with increasing $S$. However, these results were based on rather short series (six terms) and the critical point estimates contained large uncertainties.

We have re-investigated this question, using substantially longer series (14th order for $S = \frac{1}{2}$, 12th order for $S = 1$, 9th order for $S = \frac{3}{2}$). This is made possible not only by the massive increase in computing power now available, but also by the development of efficient linked-cluster expansion methods. The reader is referred to a recent review [3] for further details of this method.

The Hamiltonian is written in the form

$$H = -J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - h \sum_i S_i^z - h_s \sum_i \eta_i S_i^z \tag{1}$$

where the $\mathbf{S}_i$ are spin $S$ operators, $h$ and $h_s$ are uniform and staggered fields, with $\eta_i = \pm 1$ on respective sublattices, and the interaction is taken between nearest neighbours $\langle ij \rangle$. $J > 0$ ($<0$) corresponds to the ferromagnet (antiferromagnet). While (1) contains the form of the exchange energy for a real spin $S$ system, for comparison between different values of $S$ and, in particular, for passage to the classical limit $S \to \infty$, it is convenient to write $\tilde{J} = JS(S+1)$ and to express critical temperatures in units of $\tilde{J}/k_B$.

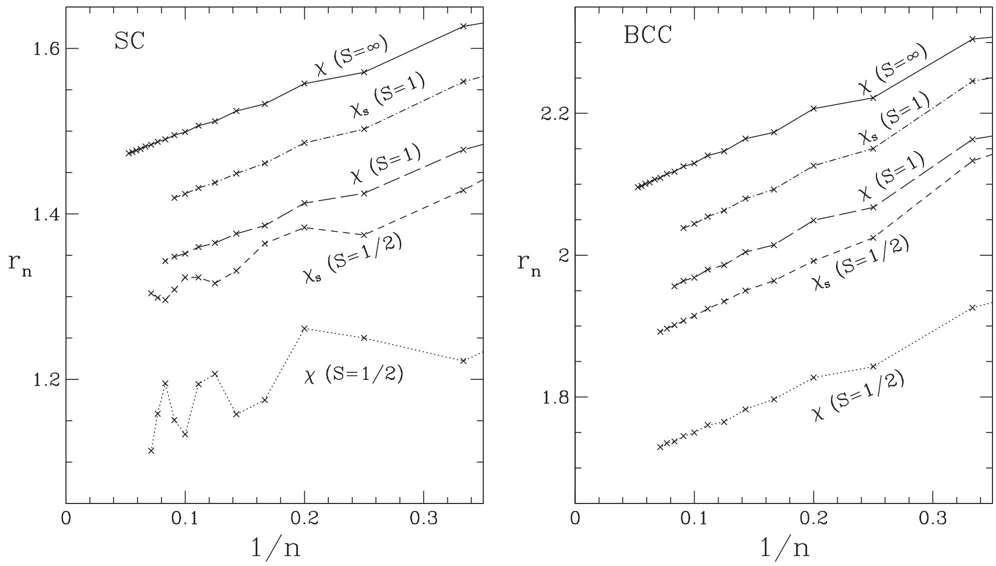


**Figure 1.** Ratio plots for the uniform and staggered susceptibilities for the SC and BCC lattices (as indicated) for $S = \frac{1}{2}, 1, \infty$. The ratios are defined for the series in the variables $\tilde{K} = JS(S+1)/k_{\mathrm{B}}T$, or equivalently $r_n = a_n/(S(S+1)a_{n-1})$ where $a_n$ are the coefficients of the series in $K$ (2).

The critical temperature $k_{\mathrm{B}}T_{\mathrm{c}}/J$ is most reliably obtained from the strongly divergent 'ordering' susceptibility in zero field: the uniform susceptibility $\chi$ for the ferromagnet or the staggered susceptibility $\chi_{\mathrm{s}}$ for the antiferromagnet. High-temperature series for these quantities can be derived in the form

$$\chi, \chi_{\mathrm{s}} = \sum_{r=0}^{\infty} a_r K^r \tag{2}$$

where $K = |J|/k_{\mathrm{B}}T$ and the $a_r$ are numerical coefficients. The uniform susceptibility for the spin $\frac{1}{2}$ case is known up to order $K^{14}$ [4], for both the SC and BCC lattices. In the present paper we give the staggered susceptibility series to the same order. This represents an addition of six new terms to the previously known series [5]. At the same time we compute uniform and staggered susceptibilities for the $S = 1$ case, up to order $K^{12}$ and $K^{11}$ respectively, for both lattices, extending the previous series by five terms. We have also calculated the corresponding series for $S = \frac{3}{2}$ up to order $K^9$. For the classical $S = \infty$ model the susceptibility series is known up to $K^{21}$ [6] and we will use this series in our comparison.

Tables 1, 3 and 2 list the series coefficients, in integer format, for both the SC and BCC lattices. The coefficients are positive and appear to be quite regular, suggesting that the radius of convergence is determined by the physical singularity on the positive real axis (we will return to this point later!). Closer inspection, however, reveals some oscillation, reflecting interference from non-physical singularities near the circle of convergence. Although we do not base our analysis on this, it is instructive to see a ratio plot [7]. We show such a plot in figure 1. Looking at the SC lattice first, it is evident that the $S = \frac{1}{2}$ series, in particular, shows a strong four-term oscillation. This results from a pair of singularities on, or near, the imaginary axis, near the circle of convergence. The $S = 1$ series are much more regular and, qualitatively, look quite similar to the $S = \infty$ case. The BCC series are rather regular, even for $S = \frac{1}{2}$. There is a two-term oscillation in all series, which is characteristic of bipartite lattices. Apart

**Table 1.** Series for $\chi$ and $\chi_s$ for spin $\frac{1}{2}$. To avoid fractions, a multiplier $4^{n+1}n!$ for $\chi$ or $4^{n+1}(n+1)!$ for $\chi_s$ has been used, where $n$ is the power of $K$.

| $n$ | $\chi$ | $\chi_s$ |
|---|---|---|
| | Simple cubic lattice $S = \frac{1}{2}$ | |
| 0 | 1 | 1 |
| 1 | 6 | 12 |
| 2 | 48 | 168 |
| 3 | 528 | 2 880 |
| 4 | 7 920 | 59 376 |
| 5 | 149 856 | 1 478 592 |
| 6 | 3 169 248 | 42 357 024 |
| 7 | 77 046 528 | 1 353 271 296 |
| 8 | 2 231 209 728 | 48 089 027 328 |
| 9 | 71 938 507 776 | 1 908 863 705 088 |
| 10 | 2 446 325 534 208 | 83 357 870 602 752 |
| 11 | 92 886 269 386 752 | 3 926 123 179 720 704 |
| 12 | 3 995 799 894 239 232 | 198 436 560 561 973 248 |
| 13 | 180 512 165 153 832 960 | 10 823 888 709 015 846 912 |
| 14 | 8443 006 907 441 565 696 | 635 114 442 481 347 244 032 |
| | Body centred cubic lattice $S = \frac{1}{2}$ | |
| 0 | 1 | 1 |
| 1 | 8 | 16 |
| 2 | 96 | 320 |
| 3 | 1 664 | 8 192 |
| 4 | 36 800 | 248 768 |
| 5 | 1 008 768 | 8 919 296 |
| 6 | 32 626 560 | 367 854 720 |
| 7 | 1 221 399 040 | 17 216 475 136 |
| 8 | 51 734 584 320 | 899 434 884 096 |
| 9 | 2 459 086 364 672 | 51 925 815 320 576 |
| 10 | 129 082 499 311 616 | 3 280 345 760 086 016 |
| 11 | 7 432 690 738 003 968 | 225 270 705 859 919 872 |
| 12 | 464 885 622 793 134 080 | 16 704 037 174 526 894 080 |
| 13 | 31 456 185 663 820 136 448 | 1 330 557 135 528 577 925 120 |
| 14 | 2284 815 238 218 471 260 160 | 113 282 648 639 921 512 955 904 |

from the $S = \frac{1}{2}$ (SC) case, reasonable estimates of the Curie and Néel temperatures can be made visually. Unless something totally unexpected occurs at higher orders, it seems clear that the Néel temperature exceeds the Curie temperature for both $S = \frac{1}{2}$ and 1 (remembering that the intercept on the ordinate axis is $k_B T_c/\tilde{J}$). The very similar limiting slopes of the different plots are consistent with the universality expectation that all quantities diverge with the same exponent $\gamma$.

To obtain more accurate estimates of the critical parameters we turn to Padé approximants [7]. Tables 4, 5 give estimates of the critical point $K_C$ and exponent $\gamma$, assuming a normal power-law singularity

$$\chi, \chi_s \sim C_0(1 - K/K_C)^{-\gamma}; \qquad K \to K_C- \tag{3}$$

obtained from high-order Padé approximants to the logarithmic derivative series. Different approximants give quite consistent results and we summarize the overall estimates of the critical temperature in table 6. The exponent estimates from the highest approximants are

**Table 2.** Series for $\chi$ and $\chi_s$ for spin 1. To avoid fractions, a multiplier $3^{n+1}n!/2$ ($3^{n+1}(n+1)!/2$) has been used for $\chi$ ($\chi_s$) series, where $n$ is the power of $K$.

| $n$ | $\chi$ | $\chi_s$ |
|---|---|---|
| Simple cubic lattice $S = 1$ | | |
| 0 | 1 | 1 |
| 1 | 12 | 24 |
| 2 | 222 | 702 |
| 3 | 5 904 | 26 280 |
| 4 | 201 870 | 1 184 526 |
| 5 | 8 556 912 | 63 357 984 |
| 6 | 426 905 802 | 3 887 604 666 |
| 7 | 24 674 144 724 | 270 348 199 128 |
| 8 | 1 616 505 223 518 | 20 988 390 679 758 |
| 9 | 118 701 556 096 392 | 1 802 403 961 243 776 |
| 10 | 9 628 527 879 611 262 | 169 418 364 565 523 958 |
| 11 | 856 813 238 084 411 136 | 17 314 303 199 655 636 792 |
| 12 | 82 856 991 914 713 902 402 | |
| Body centred cubic lattice $S = 1$ | | |
| 0 | 1 | 1 |
| 1 | 16 | 32 |
| 2 | 424 | 1 320 |
| 3 | 16 512 | 71 136 |
| 4 | 819 240 | 4 588 968 |
| 5 | 50 363 136 | 351 263 232 |
| 6 | 3 652 143 480 | 30 873 601 080 |
| 7 | 307 454 670 000 | 3 082 065 903 648 |
| 8 | 29 310 549 057 000 | 343 320 789 071 016 |
| 9 | 3 133 368 921 937 824 | 42 320 100 429 654 912 |
| 10 | 370 060 173 560 963 304 | 5 709 664 512 091 086 984 |
| 11 | 47 968 071 364 509 850 944 | 837 942 419 330 764 322 976 |
| 12 | 6756 542 767 252 059 234 840 | |

around 1.42 ($S = \frac{1}{2}$), 1.41 ($S = 1$). Early studies of the $S = \infty$ series also gave values in this range, although the recent long series give lower values, approaching the field theory prediction $\gamma \simeq 1.39$. Our results are consistent with the universality expectation.

Figure 2 shows plots of critical temperatures $k_B T_c/S(S+1)J$ versus $1/S(S+1)$. The plots appear linear, particularly if the $S = \frac{1}{2}$ points are excluded, and indicate that, to a very good approximation,

$$k_B T_c/J \sim aS(S+1) + b \tag{4}$$

where $a, b$ are constants independent of $S$. Their values are

| | SC | | BCC | |
|---|---|---|---|---|
| | $\chi$ | $\chi_s$ | $\chi$ | $\chi_s$ |
| $a$ | 1.4429 | | 2.0542 | |
| $b$ | −0.288 | −0.150 | −0.320 | −0.174 |

This linear relation may then be used to obtain reliable estimates of Curie and Néel temperature for values $S > \frac{3}{2}$.

**Table 3.** Series for $\chi$ and $\chi_s$ for spin $\frac{3}{2}$. To avoid fractions, a multiplier $2^{n+2}n!/5$ ($2^{n+3}(n+1)!/5$) has been used for $\chi$ ($\chi_s$) series, where $n$ is the power of $K$.

| $n$ | $\chi$ | $\chi_s$ |
|---|---|---|
| Simple cubic lattice $S = \frac{3}{2}$ | | |
| 0 | 1 | 2 |
| 1 | 60 | 60 |
| 2 | 1 440 | 2 220 |
| 3 | 50 136 | 106 032 |
| 4 | 2 241 660 | 6 103 230 |
| 5 | 124 125 372 | 417 121 164 |
| 6 | 8 102 868 414 | 32 715 943 017 |
| 7 | 613 292 153 184 | 2 911 926 450 048 |
| 8 | 52 599 376 466 556 | 289 263 779 556 198 |
| 9 | 5056 198 898 505 288 | 31 792 485 934 519 488 |
| Body centred cubic lattice $S = \frac{3}{2}$ | | |
| 0 | 1 | 2 |
| 1 | 80 | 80 |
| 2 | 2 720 | 4 160 |
| 3 | 136 448 | 283 776 |
| 4 | 8 751 600 | 23 240 440 |
| 5 | 696 028 496 | 2 263 139 152 |
| 6 | 65 331 028 472 | 253 095 247 076 |
| 7 | 7 121 212 898 544 | 32 175 304 799 424 |
| 8 | 879 298 191 968 624 | 4 563 926 306 507 096 |
| 9 | 121 768 840 349 153 216 | 716 734 730 963 510 496 |

**Table 4.** Estimates of the critical point $K_C$ and exponent $\gamma$ (in brackets) from $[N, D]$ Padé approximants to the spin $\frac{1}{2}$ uniform/staggered susceptibility series. Defective PAs are denoted by *.

| | Spin $S = \frac{1}{2}$ | | | |
|---|---|---|---|---|
| | Simple cubic | | Body centred cubic | |
| $[N, D]$ | F ($\chi$) | AF ($\chi_s$) | F ($\chi$) | AF ($\chi_s$) |
| [6, 7] | 1.1900 | 1.0577 | 0.7935 | 0.7266 |
| | (1.414) | (1.426) | (1.416) | (1.436) |
| [7, 6] | 1.1925 | 1.0611 | 0.7935 | 0.7266 |
| | (1.432) | (1.455) | (1.416) | (1.435) |
| [5, 7] | 1.1914 | 1.0598 | 0.7937 | 0.7266 |
| | (1.421) | (1.440) | (1.419) | (1.434) |
| [6, 6] | 1.1914 | 1.0597 | 0.7936 | 0.7264 |
| | (1.421) | (1.439) | (1.417) | (1.431) |
| [7, 5] | 1.1931 | * | 0.7939 | 0.7267 |
| | (1.438) | | (1.423) | (1.436) |
| [5, 6] | 1.1910 | 1.0592 | 0.7937 | 0.7264 |
| | (1.418) | (1.434) | (1.418) | (1.432) |
| [6, 5] | 1.1901 | 1.0583 | 0.7936 | 0.7264 |
| | (1.411) | (1.425) | (1.418) | (1.432) |

With our longer series we are also able, for the first time, to estimate values for the amplitudes $C_0$ of the leading singular term (3). This is done in two ways. The first is to use

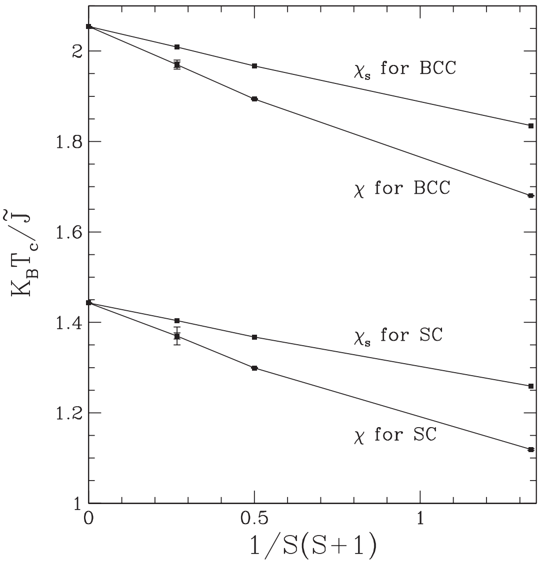


**Figure 2.** $k_B T_c/\tilde{J}$ versus $1/S(S+1)$.

**Table 5.** Estimates of the critical point $K_C$ and exponent $\gamma$ (in brackets) from $[N, D]$ Padé approximants to the spin 1 uniform/staggered susceptibility series. Defective PAs are denoted by *.

| | Spin $S = 1$ | | | |
|---|---|---|---|---|
| | Simple cubic | | Body centred cubic | |
| $[N, D]$ | F ($\chi$) | AF ($\chi_s$) | F ($\chi$) | AF ($\chi_s$) |
| [5, 6] | 0.384 78 | | 0.264 00 | |
| | (1.409) | | (1.404) | |
| [6, 5] | 0.384 78 | | 0.263 98 | |
| | (1.409) | | (1.403) | |
| [4, 6] | 0.384 78 | * | 0.263 97 | 0.254 31 |
| | (1.409) | | (1.403) | (1.405) |
| [5, 5] | 0.384 75 | * | 0.263 89 | 0.254 31 |
| | (1.408) | | (1.398) | (1.401) |
| [6, 4] | 0.384 67 | 0.365 41 | * | 0.254 10 |
| | (1.406) | (1.409) | | (1.395) |
| [4, 5] | 0.384 87 | 0.365 66 | * | 0.254 10 |
| | (1.411) | (1.417) | | (1.395) |
| [5, 4] | 0.384 83 | 0.365 65 | * | 0.253 96 |
| | (1.410) | (1.417) | | (1.390) |

the estimates of $K_C$, $\gamma$ obtained previously, form the series for

$$(1 - K/K_C)^\gamma \chi \sim C_0 + \cdots; \qquad K \to K_C-, \tag{5}$$

and evaluate Padé approximants to this series at $K_C$. The second is to compute the series for

$$\chi^{1/\gamma} = C_0^{1/\gamma}(1 - K/K_C)^{-1}. \tag{6}$$

Padé approximants to this series should have a simple pole at $K_C$ with residue $K_C C_0^{1/\gamma}$. The two methods give consistent results. We give in table 6 our best estimates and error. As usual

**Table 6.** Estimates of the critical temperatures and leading susceptibility amplitudes, from Padé approximant analysis.

| | $S=\frac{1}{2}$ | | $S=1$ | | $S=\frac{3}{2}$ | | $S=\infty$ |
|---|---|---|---|---|---|---|---|
| | F ($\chi$) | AF ($\chi_s$) | F ($\chi$) | AF ($\chi_s$) | F ($\chi$) | AF ($\chi_s$) | $\chi$ |
| | | | SC lattice | | | | |
| $K_C$ | 1.192(2) | 1.059(2) | 0.384 78(15) | 0.3656(2) | 0.195(3) | 0.190(1) | 0.693 04 |
| $k_B T_c/J$ | 0.839(1) | 0.944(2) | 2.599(1) | 2.735(1) | 5.13(8) | 5.26(3) | |
| $k_B T_c/\tilde{J}$ | 1.119(2) | 1.259(2) | 1.299 4(5) | 1.3676(7) | 1.37(2) | 1.404(7) | 1.442 9 |
| $C_0$ | 1.26(2) | 1.20(3) | 1.11(2) | 1.07(4) | | | 0.903 0 |
| | | | BCC lattice | | | | |
| $K_C$ | 0.7935(3) | 0.7266(2) | 0.2640(2) | 0.2542(2) | 0.1354(10) | 0.1327(4) | 0.486 80 |
| $k_B T_c/J$ | 1.2602(5) | 1.376(4) | 3.788(2) | 3.934(3) | 7.39(5) | 7.54(2) | |
| $k_B T_c/\tilde{J}$ | 1.6803(6) | 1.8350(5) | 1.894(1) | 1.967(1) | 1.97(1) | 2.009(6) | 2.054 2 |
| $C_0$ | 1.15(2) | 1.10(3) | 0.98(1) | 0.94(1) | | | 0.794 |

**Table 7.** Estimates of the secondary singularity, at $-K_N$ for the uniform susceptibility and at $-K_C$ for the staggered susceptibility, for the $S=\frac{1}{2}$ models on the BCC lattice.

| | $F(K)$ | | $F_s(K)$ | |
|---|---|---|---|---|
| | $K_C = 0.7936$ | $\gamma = 1.416$ | $K_C = 0.7266$ | $\gamma = 1.435$ |
| $[N, D]$ | $-K_N$(est.) | residue | $-K_C$(est.) | residue |
| [5, 7] | −0.7160 | 0.250 | −0.7993 | 0.262 |
| [6, 6] | −0.7159 | 0.250 | −0.7985 | 0.260 |
| [7, 5] | −0.7392 | 0.321 | −0.8069 | 0.284 |
| [5, 6] | −0.7189 | 0.254 | −0.7987 | 0.261 |
| [6, 5] | * | | −0.7988 | 0.261 |
| [4, 6] | −0.7111 | 0.242 | −0.7994 | 0.262 |
| [5, 5] | −0.7107 | 0.241 | −0.7985 | 0.266 |
| [6, 4] | −0.7244 | 0.275 | −0.7911 | 0.241 |

with series analysis, these are not true statistical errors but only confidence limits based on the spread of results. As can be seen from table 6, these amplitudes are all of order 1 and show a decrease of some 30% on going from $S=\frac{1}{2}$ to $\infty$, with the antiferromagnetic amplitude some 5% smaller than the ferromagnetic one.

The conclusion that the Curie temperature $T_C$ is lower than the Néel temperature $T_N$ has a puzzling consequence, as has been remarked on before [2]. Assuming that the ferromagnetic susceptibility $\chi(K)$ also has a weak, energy-like singularity at $-K_N$ ($K_N < K_C$), as is known to be the case for the Ising model, means that the radius of convergence of the series is $|K_N|$. Hence the series coefficients must, at some point, begin to alternate in sign. To check this point further we follow the procedure of Baker *et al* [8], in seeking evidence for a singularity at $-K_N$ in the uniform susceptibility, and at $-K_C$ in the staggered susceptibility. To this end we form the series for

$$F(K) = \frac{\mathrm{d}}{\mathrm{d}K}\left(\frac{\mathrm{d}}{\mathrm{d}K}\ln\chi(K) - \frac{\gamma}{K_C - K}\right) \tag{7}$$

and

$$F_s(K) = \frac{\mathrm{d}}{\mathrm{d}K}\left(\frac{\mathrm{d}}{\mathrm{d}K}\ln\chi_s(K) - \frac{\gamma}{K_N - K}\right). \tag{8}$$

The first step subtracts out the dominant physical singularity from the logarithmic derivative series. This series is expected to have a weak singularity at the corresponding Néel or Curie point. The final differentiation is to strengthen this singularity. In table 7 we show estimates of the location of this secondary singularity and the corresponding residue for the $S = \frac{1}{2}$ series on the BCC lattice. As is clear, the series $F(K)$ shows a consistent pole at $K \simeq -0.72$, consistent with the direct estimate of $K_{\mathrm{N}}$ (table 4). Similarly the series $F_{\mathrm{s}}(K)$ shows a consistent pole at $K \simeq -0.799$, consistent with the direct estimate of $K_{\mathrm{C}}$ (table 4). These numerical estimates will, of course, depend on the choice made for $K_{\mathrm{C}}$, $K_{\mathrm{N}}$, $\gamma$ in equations (7) and (8), but are found to be relatively insensitive to this choice. We have not repeated this analysis for the SC case or for $S = 1, \frac{3}{2}$.

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