High-temperature dynamics of the Ising model in a transverse field

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We derive the moments, at $T = \infty$, of the longitudinal spin-spin correlation function of the Ising model in a transverse field. The first 20 moments are obtained for the linear chain, the first 12 moments for the fcc lattice. We use a method of Nickel [J. Phys. C 7 , 1719 (1914)] to construct the relaxation function and find excellent agreement with the exact results of Capel and Perk [Physica (Utrecht) 87A, 211 (1977)] in one dimension and extremely good convergence in three dimensions. Our method of analysis provides much better convergence than methods based on truncation of the continued-fraction representation.

I. INTRODUCTION

This paper reports some new results for the dynamical properties of the Ising model in a transverse field, which is described by the Hamiltonian

$$
J = -J \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z - \Gamma \sum_i \sigma_i^x , \qquad (1)
$$

where σ^x , σ^z are Pauli spin operators and the exchange interaction is restricted to nearest neighbors.

Our motivation for this study is twofold. Firstly, the model is directly applicable to a variety of condensedmatter systems,^I including, for example, order-disorde ferroelectrics, singlet ground-state magnetic compounds, and cooperative Jahn-Teller systems. In many of these applications the σ 's are "pseudospins" which represent the states of a two-level system, and the transverse field is responsible for transitions between the levels. The second motivation is that Eq. (1) represents probably the simplest nontrivial quantum many-body system and its dynamical properties are therefore of considerable intrinsic interest.

There have been many studies of the dynamical properties of the transverse Ising model. The early work of Chock and Dagonnier² and Moore and Williams³ was based on an approximate solution of the kinetic equations for the spin-spin correlation functions. Later work $4-6$ has been based on the Mori⁷ continued-fraction representation of the longitudinal relaxation-shape function, which is defined below, with some type of truncation approximation. This approach makes use of the frequency moments of the relaxation function, which are related in a simple way to the coefficients in the short-time expansion of the spinspin correlation function. There are two difficulties with this latter approach. It is not easy to calculate the frequency moments beyond the first few, particularly at finite temperatures. The other problem is the rather ad hoc nature of the approximations which are used to terminate the continued fraction. There appears to be no way of assessing the validity of these and it is often the case, as we shall show later, that there is no systematic convergence of the approximants as more and more moments are used.

There are a number of related quantities which describe the dynamics of (1). The most fundamental is the longitudinal spin-spin correlation function,

$$
C(\vec{R},t) = \langle \sigma_{\vec{0}}^z(0)\sigma_{\vec{R}}^z(t) \rangle_T = \frac{1}{Z} \text{Tr} \left[e^{-\beta H} \sigma_{\vec{0}}^z(0)\sigma_{\vec{R}}^z(t) \right], (2)
$$

where the operators are given in the Heisenberg picture. This function can be expanded, for short times, as

$$
C(\vec{\mathbf{R}},t) = \sum_{n=0}^{\infty} \frac{i^n}{n!} \mu_n(\vec{\mathbf{R}}) t^n , \qquad (3)
$$

where the μ_n , which we refer to as "moments," depend on \overrightarrow{R} and also on temperature. Since $C(t)$ is an even function of time, only the even moments are nonzero. The dynamic-structure function $S(\vec{k}, \omega)$, which is directly measurable by neutron scattering, is defined by

$$
S(\vec{k},\omega) = \frac{1}{2\pi} \sum_{\vec{k}} \int_{-\infty}^{\infty} dt \, e^{i(\vec{k}\cdot\vec{R}-\omega t)} C(\vec{R},t) \;, \tag{4}
$$

and it is easy to see that the frequency moments of $S(k,\omega)$,

$$
\langle \omega^n \rangle_{\vec{k}} \equiv \int_{-\infty}^{\infty} \omega^n S(\vec{k}, \omega) d\omega , \qquad (5)
$$

are related to the μ_n by

$$
\langle \omega^n \rangle_{\vec{k}} = \sum_{\vec{R}} e^{i \vec{k} \cdot \vec{R}} \mu_n(\vec{R}) \,. \tag{6}
$$

The response of a system to an external disturbance is conveniently expressed in terms of the "relaxation function"

$$
F(k,\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt \, e^{i\omega t} \frac{\{\sigma_{\vec{k}}^z(0), \, \sigma_{\vec{k}}^z(t)\}}{\{\sigma_{\vec{k}}^z(0), \, \sigma_{\vec{k}}^z(0)\}} , \qquad (7)
$$

where

$$
\{A,B\} = \int_0^B \langle e^{\lambda H} A e^{-\lambda H} B \rangle_T d\lambda - \beta \langle A \rangle \langle B \rangle . \tag{8}
$$

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In the infinite-temperature limit $(\beta \rightarrow 0)$ the functions $F(\vec{k}, \omega)$ and $S(\vec{k}, \omega)$ become identical, and thus the $\langle \omega^n \rangle_{\vec{k}}$ are also the frequency moments of the relaxation function.

We have computed the moments μ_n , up to $n = 12$, for general lattices in the infinite-temperature limit. The method of calculation and a table of results are given in Sec. II. To the best of our knowledge, previous calculations have not proceeded beyond μ_6 . The other new contribution of the present work is in the method of construction of the function $F(\vec{k}, \omega)$ from the moments. Some years ago, Nickel 8 developed a method for approximating the response function of a system from a knowledge of the first few frequency moments. Although he considered a somewhat different problem, namely a dilute ferromagnet at $T=0$, the method itself is much more general and we have applied it successfully in the present study.

In Sec. III, we discuss the continued-fraction methods for approximating $F(\omega)$ as well as giving an outline of the Nickel method. In Sec. IV we consider the linear chain, for which the autocorrelation function and its Fourier 'transform are known exactly^{9,10} at $T = \infty$. This provides a test of the methods. The Nickel method gives impressively good agreement with the exact results, while the continued-fraction methods perform poorly. In Sec. V we consider the face-centered-cubic (fcc) lattice, and present an extensive set of results for both $F(\omega)$ and $C(t)$. The conclusions of the paper are summarized in Sec. VI.

II. CALCULATION OF THE MOMENTS

The moments $\mu_n(R)$ are obtained from the short time expansion of the spin-spin correlation function, Eq. (2), which at $T = \infty$ is given by

$$
C_{\vec{R}}(t) = 2^{-N} \text{Tr}(\sigma_{\vec{0}}^z e^{iHt} \sigma_{\vec{R}}^z e^{-iHt}).
$$

It follows from this that

$$
\mu_n(\vec{R}) = 2^{-N} \text{Tr}(\sigma_{\vec{0}}^z[H, \cdots [H, \sigma_{\vec{R}}^z]]), \qquad (9)
$$

where the expression involves n nested commutators. The

occurrence of these repeated commutators makes the process of calculating the μ_n very lengthy for $n > 4$. We have developed a computer program to perform the algebra and to keep track of the large number of terms, and in this way have been able to compute all of the moments up to and including μ_{12} . Such an approach was first used by Morita $¹¹$ in a study of the dynamics of the Heisenberg</sup> model.

The calculation is based on considering a set of clusters of sites, "graphs." For each graph the procedure is, briefly, as follows.

(i) Choose an initial configuration consisting of an operator σ^2 at a particular site R and unit operators at all other sites.

(ii) Carry out a commutation, using all terms in H and storing all resulting configurations.

(iii) Repeat the procedure successively, checking whether at the conclusion of each stage any configurations have a σ^z operator at site 0 and unit operators elsewhere. Such terms have a nonzero trace and, provided that all bonds of the graph have been used, give a contribution to the moment. The whole procedure is then repeated for all nonequivalent initial sites of the graph.

The graphs which contribute to the moments, through order 12, together with their contributions, are given in Appendix A. These results are independent of the particular lattice structure. To obtain the moments for a particular lattice it is only necessary to multiply each contribution by a factor which gives the number of ways of placing the graph on the lattice. We give explicit results in Table I for the wave-vector-dependent moments $\langle \omega^n \rangle_{\vec{k}}$ for the fcc lattice. It is of course difficult, in calculations of this type, to completely exclude the possibility of small errors. However, for the case of the linear chain, the known exact results¹⁰ do provide a check. For this case we have, in fact, computed the moments through μ_{20} , using our program, and they agree exactly with those obtained by expanding the exact expression. We turn now to the problem of constructing the functions $C(t)$ and $F(\omega)$ from the moments.

TABLE I. Relaxation-function moments $\langle \omega^n \rangle_{\vec{k}}$ for the transverse Ising model at $T = \infty$ on the fcc lattice. The parameter α denotes the ratio Γ/J .

 $\langle \omega^2 \rangle_{\overrightarrow{k}} = (2J)^2 \alpha^2$ $\langle \omega^4 \rangle \rightarrow = (2J)^4(12\alpha^2+\alpha^4)$ $\langle \omega^6 \rangle \rightarrow = (2J)^6(408\alpha^2 +36\alpha^4 +\alpha^6)$ $\langle \omega^8 \rangle$ _T = (2J)⁸[21792 α^2 + (3360 + 672 f_1) α^4 + 72 α^6 + α^8] $\langle \omega^{10} \rangle_{\overrightarrow{k}} = (2J)^{10} [1532928\alpha^2 + (434112+76032f_1)\alpha^4 + (21168+950f_1)\alpha^6 +120\alpha^8 + \alpha^{10}]$ $\left(\omega^{12}\right)^{3}_{\vec{k}} = (2J)^{12}$ [130179072 α^{2} + (66 949 560 + 22 726 656 f_1) α^{4} +(6203 952 + 1864 896 f_1 + 9504 f_2 + 6336 f_3) α^6 + (152 352 + 96 096 f_1) α^8 + 180 α^{10} + α^{12}] with $f_1(\vec{k}) = \frac{1}{3} \left[\cos \frac{k_x a}{2} \cos \frac{k_y a}{2} + \cos \frac{k_x a}{2} \cos \frac{k_z a}{2} + \cos \frac{k_y a}{2} \cos \frac{k_z a}{2} \right]$ $\frac{1}{3} \left[\cos \frac{k_x a}{2} \cos \frac{k_y a}{2} + \cos \frac{k_x a}{2} \cos \frac{k_z a}{2} + \cos \frac{k_y a}{2} \cos \frac{k_z a}{2} \right]$ $f_2(\vec{k}) = \frac{1}{3} (\cos k_x a + \cos k_y a + \cos k_z a)$ $f_3(\vec{k}) = \frac{1}{3} \left[\cos k_x a \, \cos \frac{k_y a}{2} \cos \frac{k_z a}{2} + \cos \frac{k_x a}{2} \cos k_y a \, \cos \frac{k_z a}{2} + \cos \frac{k_x a}{2} \cos \frac{k_y a}{2} \cos k_z a \right]$

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III. METHODS FOR CONSTRUCTING $F(\omega)$

The Mori⁷ continued-fraction formalism expresses the Laplace transform of the time-dependent relaxation function,

$$
\widehat{F}(s) = \int_0^\infty e^{-st} F(t) dt \tag{10}
$$

as a continued fraction

$$
\hat{F}(s) = \frac{1}{s + \frac{\delta_1}{s + \frac{\delta_2}{s + \dots}}} = \frac{1}{s + \delta_1 \hat{K}_1(s)}\tag{11}
$$

with

$$
\widehat{K}_n(s) = [s + \delta_{n+1} \widehat{K}_{n+1}(s)]^{-1} ,
$$

and where the δ coefficients are directly expressible in terms of the moments $\langle \omega^n \rangle^{7,12}$ The relaxation function $F(\omega)$ is then given by

$$
F(\omega) = \frac{1}{\pi} \text{Re}\hat{F}(s = i\omega) \tag{12}
$$

Note that in the above equations, and in the remainder of this section, we suppress the \vec{k} dependence of various quantities.

Several methods of terminating the continued fraction have been proposed and are widely used in the literature. The "*n*-pole approximations" neglect the s dependence of $\hat{K}_n(s)$ and write

$$
\widehat{K}_{n-1}(s) = (s + \tau_{n-1}^{-1})^{-1} ,
$$

where τ represents a relaxation time, which is then expressed in terms of the lower-order moments. There is no unambiguous way to do this and several expressions have been used. The three-pole approximation of Lovesey and Meserve,¹³ used in much of the literature, mainly in connection with Heisenberg systems, consists of taking $\tau_2^{-2} = \frac{1}{2}\pi\delta_2$. In an earlier study of the transverse Ising model, Tommet and Huber⁵ use

$$
\tau_2^{-2} = \frac{1}{2} \pi \left[(\delta_2^{3/2} + \frac{1}{2} \delta_1^2 \delta_2^{-1/2}) / (\delta_1 + \delta_2) \right]^2.
$$

More recently, De Raedt and De Raedt¹⁴ have proposed
the ansatz $\tau_n^{-2} = \delta_{n-1} + \delta_n$, and this latter form has been used in a study of the one-dimensional transverse Ising model by Plascak et al.¹⁵

An alternative truncation approach, known as "Gaussian termination," has been used in studies of Heisenberg systems, $16-18$ and was used by Pak⁶ in his work on the transverse Ising model. In this approach the nth-order memory function $K_n(t)$ is assumed to be a Gaussian, the width of which is determined by the $(n+1)$ th moment. This leads to automatic termination of the continued fraction and an explicit expression for the function $F_n(\omega)$.¹⁸

The Nickel method is quite different from the scheme described above. Letting $s = iz$ with $\text{Im}z < 0$ in (10), using the relation

$$
F(t) = \int_{-\infty}^{\infty} d\omega' e^{i\omega' t} F(\omega') , \qquad (13)
$$

and carrying out the integral over t we have

$$
-i\widehat{F}(iz) \equiv \widetilde{F}(z) = \int_{-\infty}^{\infty} d\omega' \frac{F(\omega')}{\omega' - z} , \qquad (14)
$$

where $\tilde{F}(z)$ is an analytic function of z in the lower halfplane. If we now let $z = \omega - i\epsilon$, then as $\epsilon \rightarrow 0$ we obtain

$$
\widetilde{F}(\omega) = \sum_{n} \frac{\langle \omega^{n} \rangle}{\omega^{n+1}} - i\pi F(\omega) . \tag{15}
$$

Thus $F(\omega) = -1/\pi \text{Im}\widetilde{F}(\omega)$ and **Contract Contract**

$$
\sum_{n=0}^{\infty} \frac{\langle \omega^n \rangle}{\omega^{n+1}} = \text{Re}\,\widetilde{F}(\omega) \tag{16}
$$

A direct approximation of the moment series by Padé approximants is doomed to failure as one obtains only a set of poles (usually on the real z axis) which represents the branch cut along this axis. The imaginary piece of $\tilde{F}(\omega)$ is simply a set of δ functions rather than the continuous function which we wish to obtain.

In order to circumvent this difficulty, Nickel⁸ first carried out a nonlinear transformation

$$
\omega = \zeta + \lambda^2/\zeta \tag{17}
$$

where 2λ is the length of the branch cut on the Rez axis which is here assumed to be centered at $\omega = 0$. In the complex ζ plane the branch cut is mapped onto the circle of radius λ . The interior of the circle contains the unphysical sheet of $\widetilde{F}(\omega)$ to which any spurious singularities are confined. The exterior of the circle is the physical sheet. The transformation (17), when substituted in the moment series, increases the radius of convergence of the series. Moreover, Padé approximants to the series in $1/\zeta$ do not have poles on the branch cut and one obtains continuous real and imaginary parts of the function $F(\omega)$ in the range $-2\lambda < \omega < 2\lambda$.

At first sight it might seem that this method is limited to systems in which the branch cut is of finite extent. However, since $F(\omega)$ decreases rapidly as a function of ω , we expect that a finite series of moments will primarily produce poles in the region in which $F(\omega)$ is large. We have found this to be the case. In our analysis we first construct $\lceil N/N \rceil$ or $\lceil N/N+1 \rceil$ Padé approximants to the series, Eq. (16). The location of all poles is determined and an initial choice of λ is taken to be the location of the pole farthest from the origin. The nonlinear transformation is then carried out for a number of values of λ in the vicinity of the initial choice and the value which produces the best internal convergence of a series of approximants using more and more moments is then adopted as the final choice.

One slight disadvantage to the Nickel method is that $F(\omega) \rightarrow 0$ at $|\omega| = 2\lambda$ and, indeed, approaches zero with the functional dependence $(2\lambda - |\omega|)^{1/2}$. Since $F(\omega)$ is already quite small at this value of ω , this is not a serious problem.

IV. THE LINEAR CHAIN

For the linear chain at $T = \infty$ only the correlation function with \vec{R} = 0 is nonvanishing. Consequently the struc-

FIG. 1. Relaxation function $2\Gamma F(\omega)$ as function of $\omega/2\Gamma$ for the linear chain for (a) $\Gamma/J = 0.5$, (b) $\Gamma/J = 1.0$, and (c) $\Gamma/J = 2.0$. In each case the solid curve is the exact result of Capel and Perk (Ref. 10). Dashed curves are obtained from the Nickel method with (a) λ = 2.5, (b) λ = 2.0, and (c) λ = 1.0. [4,4] Padé approximant, intermediate length dash; [4,5] Padé approximant, short dash; [5,5] Padé approximant, long dash.

FIG. 2. Autocorrelation function $C(\tau)$ as function of $\tau \equiv 2\Gamma t$ for the linear chain for (a) $\Gamma/J = 0.5$, (b) $\Gamma/J = 1.0$, and (c) $\Gamma/J = 2.0$. Solid curve is the exact result of Capel and Perk. Dashed curves correspond to numerical integrals [Eqs. (13)] of the function $F(\omega)$ shown in Fig. 1. [4,4] Padé approximant, intermediate length dash; [4,5] Padé approximant, short dash; [5,5] Padé approximant, long dash.

FIG. 3. Relaxation function $2\Gamma F(\vec{k}\omega)$ at $\vec{k}=\vec{0}$ for the fcc lattice as determined by the Nickel method. (a) $\Gamma/J=1.0$, $\lambda=3.0$; (b) $\Gamma/J = 3.0, \lambda = 2.35$; (c) $\Gamma/J = 6.0, \lambda = 1.8$. [1,2] Padé approximant, dotted curve. The [2,2], [2,3], and [3,3] Padé approximants are almost indistinguishable. The solid curve is the [3,3] Padé approximant.

FIG. 4. Relaxation function $2\Gamma F(\vec{k},\omega)$ at $\vec{k}=\vec{0}$ for the fcc lattice obtained by Gaussian truncation of the continued fraction representation for (a) $\Gamma/J = 1.0$, (b) $\Gamma/J = 3.0$, and (c) $\Gamma/J = 6.0$. First-order approximation, dotted curve; second-order approximation, short dashes; third-order approximation, chain dot; fourth-order approximation, long dashes; fifth-order approximation, solid line.

FIG. 5. Relaxation function $2\Gamma F(\vec{k},\omega)$ at $\vec{k}=\vec{0}$ for the fcc lattice obtained by the de Raedt approximation scheme of the contin- $= 3.0$, and (c) $\Gamma/J = 6.0$. First-order truncation, dotted curve; second-order truncation, short es; third-order truncation, chain dot; fourth-order truncation, long dashes; fifth-order truncation, solid line. The fourth- and fifth-order curves in 2(a) are not distinguishable.

FIG. 6. Autocorrelation function $C(\vec{k}, \tau)$ at $k = 0$ for the fcc lattice where $\tau = 2\Gamma t$. $C(\vec{k}, \tau)$ is obtained by Fourier transform of the functions $F(\vec{k}, \omega)$ plotted in Fig. 3. Again only the transform of the [1,2] Padé approximant deviates significantly from the converged result. (a) $\Gamma/J = 1.0$, (b) $\Gamma/J = 3.0$, and (c) $\Gamma/J = 6.0$.

ture function and relaxation function are independent of wave number. Capel and Perk¹⁰ have calculated $C(t)$ and $F(\omega)$ exactly for general values of the parameters Γ, J . Both functions consist of a Gaussian multiplied by a Jacobi θ function. For the special case $\Gamma = J$ the functions are pure Gaussian.⁹ We have generated the moments through μ_{20} for this case and have used these to test the accuracy of the Nickel method. In Fig. ¹ we show results for the relaxation function $F(\omega)$, for three values $\Gamma/J=0.5$, 1.0, and 2.0, obtained from the higher-order Pade approximants. Agreement with the exact results is remarkably good. Also gratifying is the fact that higher-order Fade approximants, which make use of more moments, give more accurate results. We have also computed $F(\omega)$ from the continued-fraction representation using both De Raedt n-pole and Gaussian termination. In both cases low-order approximants tend to give an $F(\omega)$ with the correct qualitative shape, but with quite incorrect numerical values. Higher-order approximants contain totally spurious structure and show no indication of convergence. This type of behavior, in the case of the isotropic Heisenberg ferromagnet, has already been noted by Tucker.¹⁸

From the approximants for $F(\omega)$ we have computed $C(t)$ by simple numerical integration. These results are shown in Fig. 2, as are the exact results. The agreement is again excellent.

V. THE FCC LATTICE

We have also analyzed the moment series for the transverse Ising model on the fcc lattice using the three aforementioned methods. We have calculated the relaxation function $F(\vec{k}, \omega)$ at the zone center $(\vec{k} = \vec{0})$ and at the zone boundary point $\vec{k}=(\pi/a)(1,1,1)$. As there is very little difference between the results for these two values of \vec{k} we report only the results for $\vec{k} = \vec{0}$. In Figs. 3(a)–3(c) we display the relaxation function for $\Gamma/J=1$, 3, and 6 determined from the [1,2], [2,2], [2,3], and [3,3] Pade approximants to the moment series after it has been transformed according to Eq. (17). Except for $\Gamma/J=3$, the internal convergence of the approximants is remarkably good and at $\Gamma/J=3$ it is only the lowest-order [1,2] approximant which shows any significant deviation from the others. In the vicinity of this value of Γ/J the relaxation function changes from one with only a central peak to one with a peak at a nonzero value of ω and it may be that this crossover is only properly reflected in the higher moments. In Figs. $4(a) - 4(c)$ and $5(a) - 5(c)$ we display the

results obtained using Gaussian and De Raedt termination of the continued fraction. As in the case of the linear chain, the first three approximants in each of the schemes seem to converge to a function similar to that obtained from the Nickel method. The higher-order approximants are quite different and there is no indication that these procedures will converge at all. In Figs. 6(a)—6(c) we plot the autocorrelation function for the same values of Γ/J at $\vec{k}=\vec{0}$ obtained by evaluating the integral, Eq. (13), between -2λ and 2λ with $F(\omega)$ determined by the Nickel method. Because of the cutoff at 2λ , which is inherent in the Nickel method, there are some spurious truncation oscillations. These are, however, too small to show up on the scale of the graphs. The convergence of $C(t)$ is seen to be extremely good.

VI. CONCLUSIONS

We have derived the frequency moments at $T=\infty$ through order 12 of the relaxation function of the transverse Ising model in three dimensions and through order 20 for the linear chain. We have shown that the relaxation function can be reconstructed very accurately using a method of Nickel.⁸ The agreement with the exact onedimensional results of Capel and $Perk^{10}$ is extremely good and in three dimensions the internal convergence of the results is quite impressive. Since even low-order approximants in three dimensions display the correct behavior, we believe that there is reason to be optimistic that the dynamics of other quantum many-body systems can be determined in the same way.

The relaxation function of the transverse Ising model seems to be a smooth nonsingular function of ω for all values of Γ/J . It will be of considerable interest to study the relaxation function of systems such as the spin- $\frac{1}{2}$ Heisenberg antiferromagnetic chain which is believed to diverge at $\omega=0$. Preliminary results for this problem are encouraging and are planned to be reported in a separate paper.

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APPENDIX

The graphs which contribute to the moments, through order 12, are shown below. The contribution of a particular graph and a particular choice of initial and final sites (IF) is expressed as a sum of terms of the form $C(m, n)$. This denotes a contribution to μ_{m+n} of the form $\mathbb{C}J^m\Gamma^n$.

	Graph	(IF)	Contribution	
G,		(1,1)	$1(0,2) + 1(0,4) + 1(0,6) + 1(0,8) + 1(0,10) + 1(0,12) + \cdots$	
G,	2	(1,1)	$1(2,2) + 1(4,2) + 3(2,4) + 1(6,2) + 5(4,4) + 6(2,6)$ $+1(8,2)+7(6,4)+15(4,6)+10(2,8)+1(10,2)$ $+9(8,4) + 28(6,6) + 35(4,8) + 15(2,10) + \cdots$	

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