量子統計の進歩

理論研究40年を振り返って

1. 熱力学ベーテ仮説方程式（１９７０－）
2. 低次元系スピン波理論の定式化（１９８６－１９９０）
3. 量子モンテカルロ法の物性物理への応用（１９８４－１９９０）
4. ４体力スピン相互作用の導出（１９７７）
5. 有機強磁性体の研究（１９９１－１９９５）
6. 一次元磁性体の研究（１９７０－）
7. 可解模型の相関関数の研究（１９７７－

		Supervisor	Main interest
1967	東大大学院	久保先生	
68			Hubbard model
69			Thermodynamic Bethe ansatz
70			
71			
72	大阪大学	西山先生	
73			1D delta Boson
74			
75			
76	CNRS Grenoble	Prof.M.Cyrot	Strong coupling expansion
77			

	助手	院生	客員	PD
1978				
79				
80				
81	今田			
82				
83		山田		
84				
85		野村		
86	常次	宮里		
87		坂井		
88				
89				
90		中村、矢島		
91		中野		
92	河原林	河野、河野、塚野		
93		岩崎		Manning
94		伊藤	Kusmartsev	
95		村本、玉井	Inozemtsev	Williams
96				
97				
98				中村
99				
2000	城石			
1		佐藤		
2				堺
3				坪井
4				
5			Boos	
6				
7				

１９６８　Lieb-Wuによる１次元Hubbard模型の厳密解

磁化曲線および磁化率の計算

$$\mathscr{H} = -T \sum_{\langle ij \rangle} \sum_{\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + I \sum_{i=1}^{N_a} c_{i\uparrow}^{\dagger} c_{i\uparrow} c_{i\downarrow}^{\dagger} c_{i\downarrow}; \quad T > 0,$$

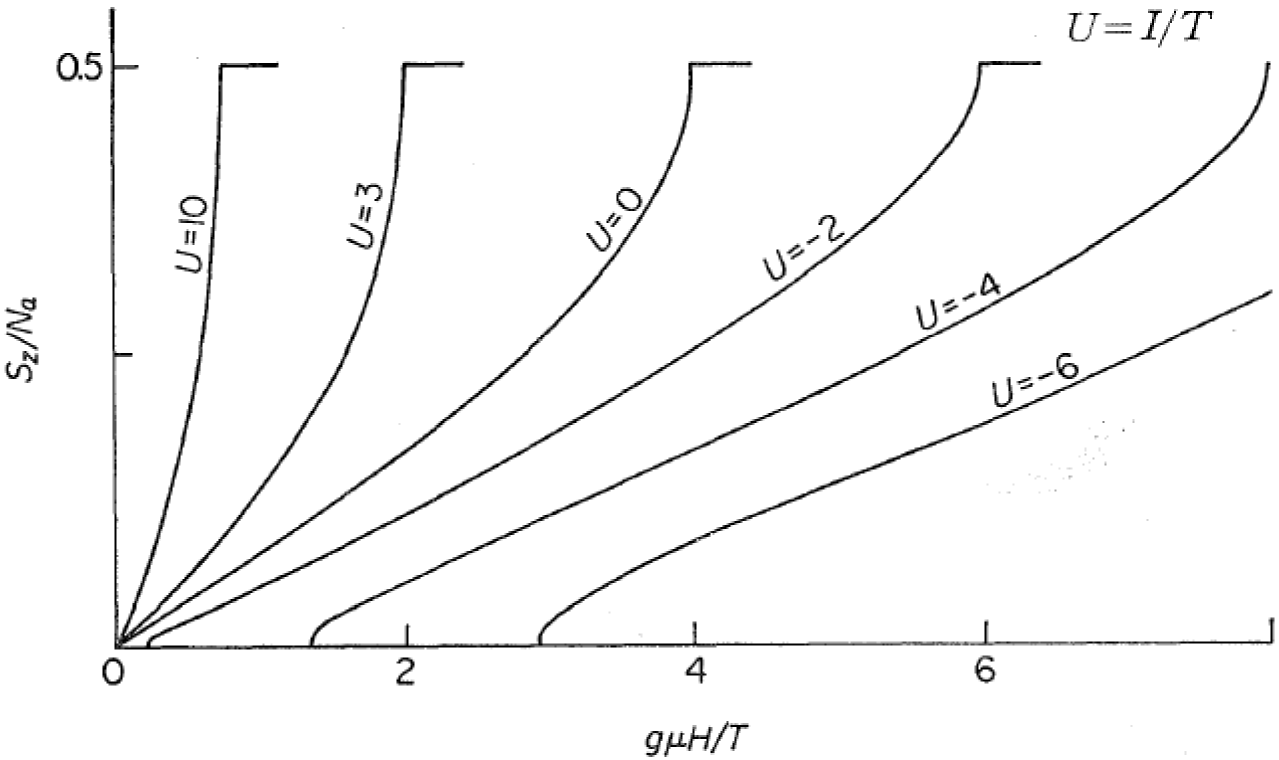


Fig. 2. The magnetization as a function of magnetic field for the one-dimensional half-filled Hubbard model at zero temperature.

Minoru Takahashi, Prog. Theor. Phys. 42, 1098-1105 (1969) ‡

$$\chi = \frac{\mu_0^2}{\pi T} I_0\left(\frac{2\pi}{U}\right) \Big/ I_1\left(\frac{2\pi}{U}\right).$$

$$U = I/T$$

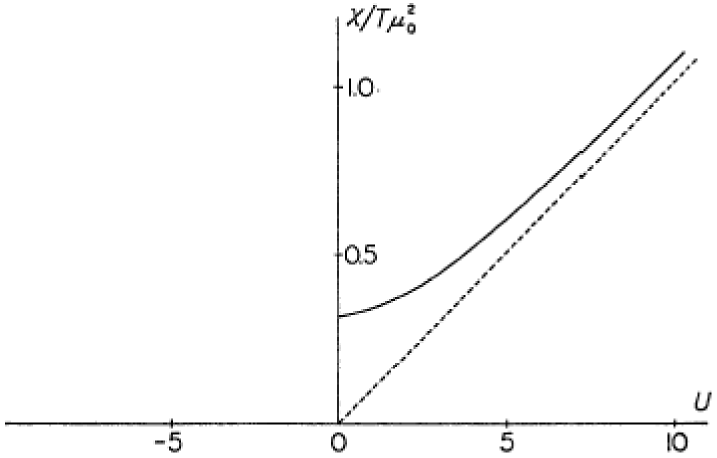
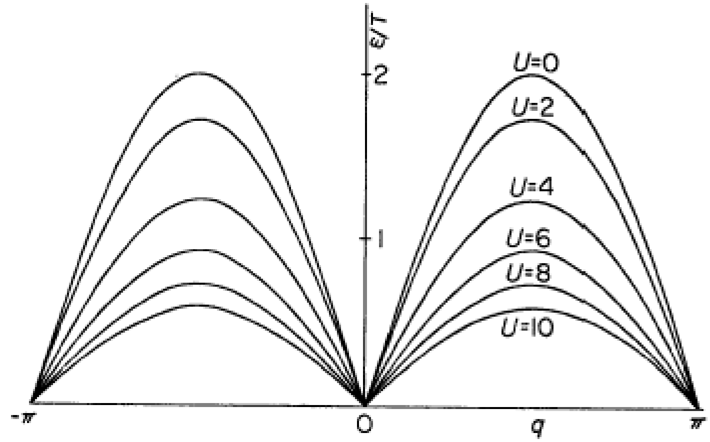


Fig. 1. Magnetic susceptibility χ is plotted vs $U=I/T$. In the case $U<0$ χ is zero. The dashed line is the asymptote at $U\to\infty$.



$$v_s = \left|\frac{d\varepsilon}{dq}\right| = 2T I_1\left(\frac{2\pi}{U}\right) \Big/ I_0\left(\frac{2\pi}{U}\right).$$

$$\chi = \frac{2\mu_0^2}{\pi v_s}.$$

Minoru Takahashi, Prog. Theor. Phys. 43, 1619 (1970) ‡

絶対零度での可解模型の基底状態エネルギーはBethe ansatz解の分布関数で決まる。

XXX模型・・・Hulthen １９３８

XXZ模型・・・Orbach, Walker　１９５８，１９５９

XYZ模型・・・Baxter 1972

δBoson・・・Lieb-Liniger 1963

δFermion(s=1/2)・・・Gaudin, Yang 1967

δFermion(s>1/2, c>0)・・・Sutherland 1968

δFermion(s>1/2, c<0)・・・Takahashi, Yang 1970

1D Hubbard model・・・Lieb-Wu 1968

Fredholm type linear integral equation

$$\mathcal{H} = J \sum_{i=1}^{N} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z - \tfrac{1}{4})$$

$$\mathbf{S}_{N+1} = \mathbf{S}_1 .$$

$$e^N(\Lambda_j) = \prod_{\substack{l \neq j \\ l=1}}^{M} e\left(\frac{\Lambda_j - \Lambda_l}{2}\right), \qquad j = 1, 2, \cdots, M ,$$

where $e(x) = (x+i)/(x-i)$.

Conjecture 1. Complex Λ always forms a bound state with several other Λ's. For a bound state of n-Λ's the real parts of Λ's are the same and the imaginary parts are $(n-1)i$, $(n-3)i$, $\cdots$ $-(n-3)i$ and $-(n-1)i$ within the accuracy of $O(\exp(-\delta N))$, $\delta > 0$.

Minoru Takahashi, Prog. Theor. Phys. 46, 401-415 (1971) ‡

$$\mathcal{H} = -\sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2} + 4c \sum_{i<j} \delta(x_i - x_j) + \mu_0 H(2M - N),$$

$$e^{ik_jL} = \prod_{\alpha=1}^{M} e\left(\frac{k_j - \Lambda_\alpha}{c}\right),$$

$$\prod_{j=1}^{N} e\left(\frac{\Lambda_\alpha - k_j}{c}\right) = \prod_{\beta \neq \alpha} e\left(\frac{\Lambda_\alpha - \Lambda_\beta}{2c}\right).$$

Conjecture 1. If a set of solutions $(k_1, k_2, \cdots, k_N; \Lambda_1, \Lambda_2, \cdots, \Lambda_M)$ of (2·8) and (2·9) contain a complex k (or Λ), $\bar{k}$ (or $\bar{\Lambda}$) is also contained in the set of k's (or Λ's).

Conjecture 2. Complex Λ always forms a bound state with several other Λ's. In this set of Λ's the real parts of these Λ's are the same and the imaginary parts are $(n-1)ci$, $(n-3)ci$, $\cdots$, $-(n-1)ci$ for the bound state of $n-\Lambda$'s within the accuracy of $O(\exp(-\delta N))$, where δ is a positive number.

Conjecture 3. In the case $c<0$, complex k_α makes a pair with its complex conjugate $\bar{k}_\alpha$ and a real Λ, which we write as Λ_α'. The real parts of k_α, $\bar{k}_\alpha$ and Λ_α' are the same and the imaginary parts of k_α and $\bar{k}_\alpha$ are c and $-c$ within the accuracy of $O(\exp(-\delta L))$.

Minoru Takahashi, Prog. Theor. Phys. 46, 1388-1406 (1971) ‡

$$\mathcal{H} = -\sum_{\langle ij\rangle}\sum_{\sigma} c^{\dagger}_{i\sigma}c_{j\sigma} + 4U\sum_{i=1}^{N} n_{i\uparrow}n_{i\downarrow} - \sum_{i=1}^{N}\mu_0 H(n_{i\uparrow} - n_{i\downarrow}).$$

$$\exp(ik_j N_a) = \prod_{\alpha=1}^{M} e\left(\frac{\sin k_j - \Lambda_\alpha}{U}\right),$$

$$\prod_{j=1}^{N} e\left(\frac{\Lambda_\alpha - \sin k_j}{U}\right) = -\prod_{\beta=1}^{M} e\left(\frac{\Lambda_\alpha - \Lambda_\beta}{2U}\right),$$

Conjecture 1. A complex k_j belongs to a pair of electrons or a bound state of pairs. For a bound state of n-pairs there are $n-\Lambda$'s which have the same real part and the imaginary parts as $(n-1)iU$, $(n-3)iU, \cdots -(n-1)iU$ within the accuracy of $O(\exp -\delta N_a)$, where δ is some positive number. And $2n-k$'s belong to this bound state and take the values

$$\begin{aligned}
k_\alpha^{1} &= \pi - \sin^{-1}(\Lambda_\alpha'^{n} + niU),\\
k_\alpha^{2} &= \sin^{-1}(\Lambda_\alpha'^{n} + (n-2)iU),\\
k_\alpha^{3} &= \pi - k_\alpha^{2},\\
k_\alpha^{4} &= \sin^{-1}(\Lambda_\alpha'^{n} + (n-4)iU),\\
k_\alpha^{5} &= \pi - k_\alpha^{4},\\
&\ \vdots\\
k_\alpha^{2n-2} &= \sin^{-1}(\Lambda_\alpha'^{n} - (n-2)iU),\\
k_\alpha^{2n-1} &= \pi - k_\alpha^{2n-2},\\
k_\alpha^{2n} &= \pi - \sin^{-1}(\Lambda_\alpha'^{n} - niU),
\end{aligned} \qquad (2\cdot 9\mathrm{a})$$

within the accuracy of $O(\exp(-\delta N_a))$. Here we put $-\pi/2 < \mathrm{Re}\sin^{-1}(x) \leqq \pi/2$.

Conjecture 2. Complex Λ belongs to a bound state of pairs or bound state of Λ's. In the latter case the real parts of Λ's are the same and the imaginary parts are $(n-1)iU$, $(n-3)iU, \cdots, -(n-1)iU$ within the accuracy of $O(\exp -\delta N)$.

Minoru Takahashi, Prog. Theor. Phys. 47, 69-82 (1972) ‡

$$\left\{\frac{\operatorname{sh}\frac{1}{2}\theta(x_\alpha+i)}{\operatorname{sh}\frac{1}{2}\theta(x_\alpha-i)}\right\}^N=-\prod_{\beta=1}^{M}\left\{\frac{\operatorname{sh}\frac{1}{2}\theta(x_\alpha-x_\beta+2i)}{\operatorname{sh}\frac{1}{2}\theta(x_\alpha-x_\beta-2i)}\right\};\quad \alpha=1,2,\cdots M.$$

Assumption 1: A string of order n consists of the sets

$$x_{\alpha,+}^{n,k}\equiv x_\alpha{}^n+(n+1-2k)i+O(\exp-\delta N) \qquad (\mathrm{mod}\ 2p_0 i)$$

and

$$x_{\alpha,-}^{n,k}\equiv x_\alpha{}^n+(n+1-2k)i+p_0 i+O(\exp-\delta N), \quad (\mathrm{mod}\ 2p_0 i) \qquad (2\cdot 9)$$

where $\delta>0$, $k=1,2,\cdots,n$, and $x_\alpha{}^n$ is real. We call these states the n-th-order bound states with $+$ and $-$ parities, respectively.
Assumption 2: The parity v and order n of a bound state should satisfy the following conditions:

$$\sin\{\pi(n-1)/p_0\}\geq 0 \quad \text{for} \quad v=+1, \qquad (2\cdot 10\mathrm{a})$$

$$\sin\{\pi(n-1)/p_0\}\leq 0 \quad \text{for} \quad v=-1 \qquad (2\cdot 10\mathrm{b})$$

and

$$2\sum_{j=1}^{n-1}[j/p_0]=(n-1)[(n-1)/p_0], \qquad (2\cdot 11)$$

Hida, K. (1981) Phys. Lett. 84A,338.

Fowler, M. and Zotos, X.(1981) Phys. Rev. B 24,2634.

Minoru Takahashi and Masuo Suzuki, Prog. Theor. Phys. 48, 2187-2209 (1972) ‡

１９６９　Yang-Yangによる１次元デルタ関数Bosonの熱力学

・・・・１個の未知関数を含む非線形積分方程式

１９７１　Gaudin -Takahashi equation,　|Δ|≧0, Λ string

・・・・無限個の未知関数を含む非線形積分方程式

１９７２　１次元デルタ関数Ｆｅｒｍｉｏｎの熱力学、１次元Hubbard
　　模型の熱力学方程式(k-Λ　string)

Δ＝cos π/nの時n-1個の未知関数を持つ積分方程式

Δ＝cos π* rational numberのとき有限個の未知関数を持つ。

XXZとXYZ模型の熱力学方程式の完成

・・・Takahashi-Suzuki equation

Yang-Yang type non-linear integral equation

Low-temperature thermodynamics of 1D Hubbard

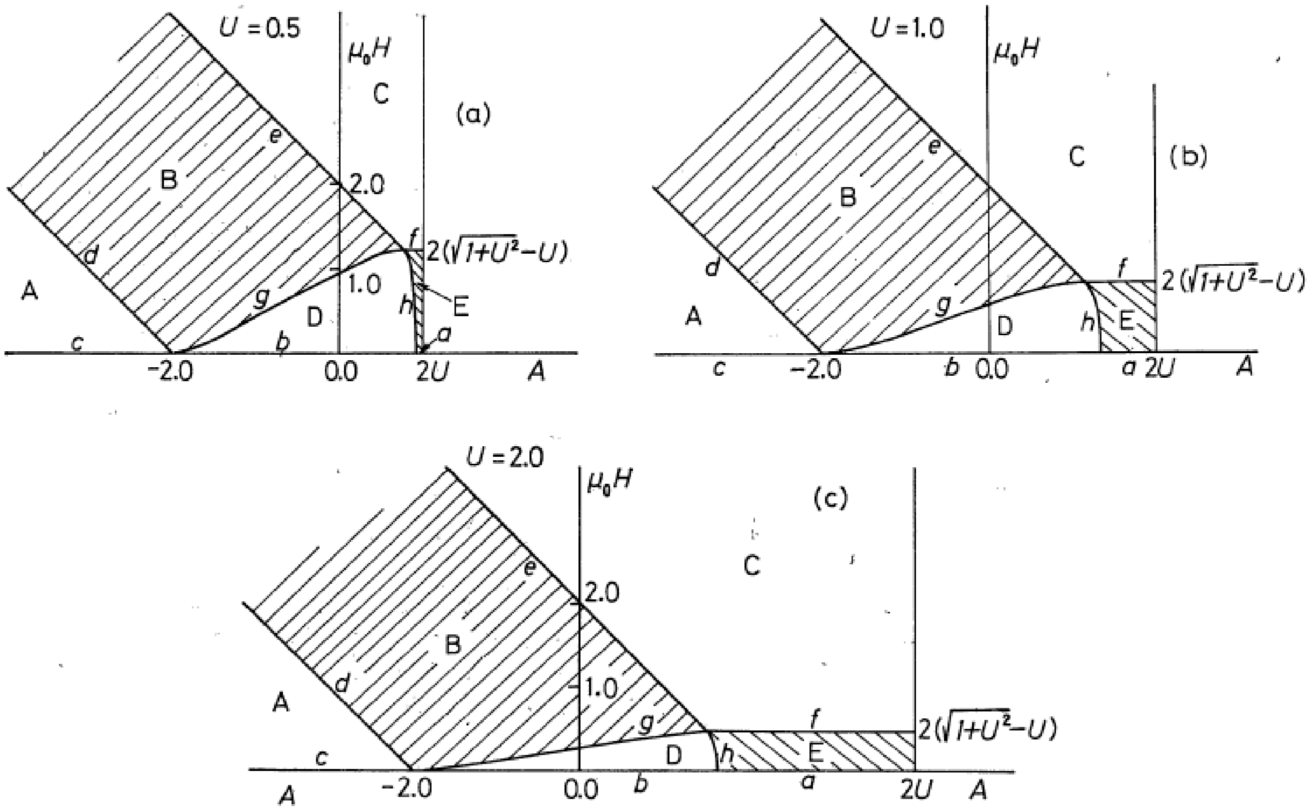


Fig. 1. Characteristic regions of low-temperature specific heat for various values of U. On lines d, e, f, g and h, low-temperature specific heat is proportional to $T^{1/2}$. In regions B, D and E, it is proportional to T. In regions A and C, it is proportional to $T^{-3/2}\exp(-\alpha/T)$.

a) $U=0.5$
b) $U=1.0$
c) $U=2.0$

Minoru Takahashi, Prog. Theor. Phys. 52, 103-114 (1974) ‡

Low-temperature thermodynamics of XXZ and XYZ chain

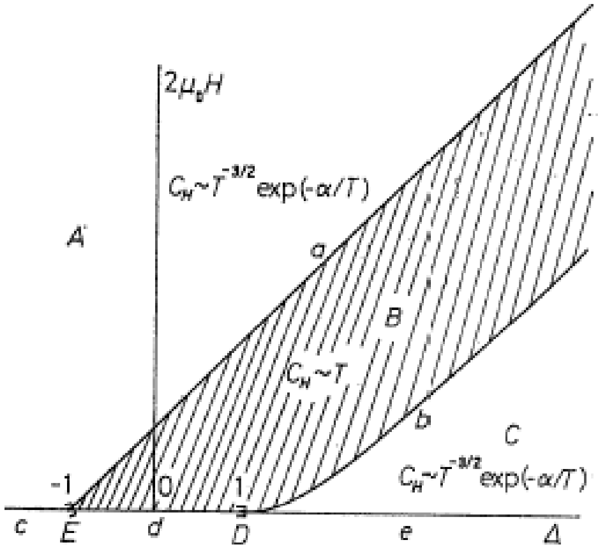


Fig. 2.

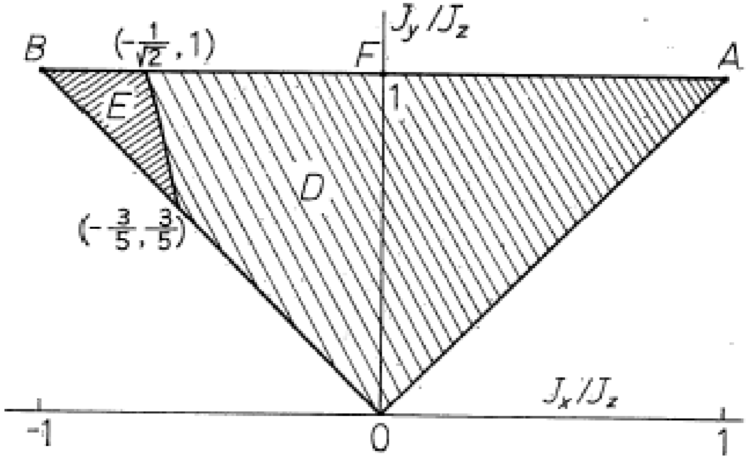


Fig. 3.

Fig. 2. Properties of the low-temperature specific heat of the Heisenberg-Ising model at $J=+1$. Regions A, B, C contain neither lines a, b, c, d, e nor end points D, E. Point D is contained in line d and point E is contained in line c.

Fig. 3. Properties of the low-temperature specific heat of the X-Y-Z model in zero field.

Minoru Takahashi, Prog. Theor. Phys. 50, 1519-1536 (1973) ‡

$$\lim_{H\to 0}\lim_{T\to 0} C_H/T = \frac{2\theta}{3J\sin\theta}.$$

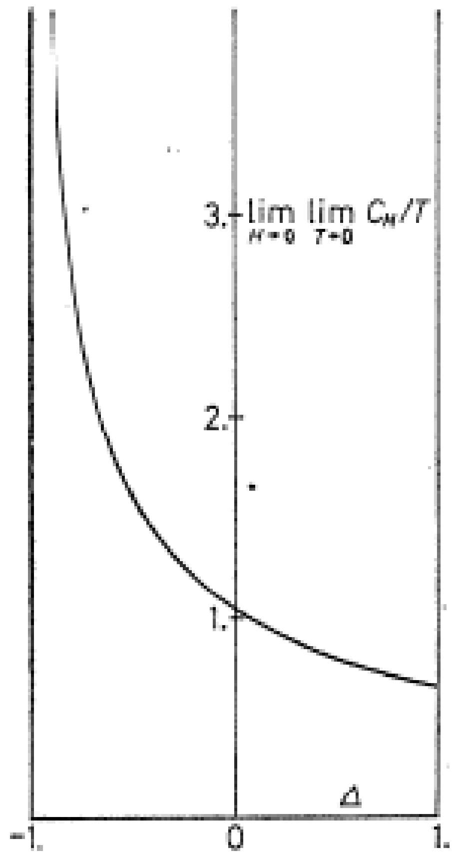


Fig. 1. The coefficient of T-linear low-temperature specific heat in the limit $T\to 0$ and $H\to 0$. In the limit $\Delta\to -1$, $\lim_{H\to 0}\lim_{T\to 0} C_H/T$ diverges as $(1+\Delta)^{-1/2}$.

Table II. Analytic expression of physical quantities at $J>0$ and $0\le\theta<\pi$.

$\lim_{H\to 0}\lim_{T\to 0}\chi$	$\lim_{H\to 0}\lim_{T\to 0} C_H/T$	The ground state energy per site
$\frac{4\theta\mu_0^2}{J(\pi-\theta)\pi\sin\theta}$	$\frac{2\theta}{3J\sin\theta}$	$-J\sin\theta\int_{-\infty}^{\infty}\frac{\mathrm{sh}(\pi-\theta)\omega\, d\omega}{2\,\mathrm{ch}\,\theta\omega\,\mathrm{sh}\,\pi\omega}$

Minoru Takahashi, Prog. Theor. Phys. 50, 1519-1536 (1973) ‡

Ferromagnet at Low-Temperature

Using Bethe ansatz integral equations, we calculate the free energy and susceptibility of spin-$\frac{1}{2}$ one-dimensional Heisenberg ferromagnet $\mathscr{H}=J\sum(\boldsymbol{S}_i\boldsymbol{S}_{i+1}-\frac{1}{4})$, $(J<0)$ at $T\geq 0.004|J|$. We find that the free energy and susceptibility are expanded by $\sqrt{T/|J|}$ at low temperature:

$$f=|J|\left\{-1.042\left(\frac{T}{|J|}\right)^{3/2}+1.00\left(\frac{T}{|J|}\right)^{2}-0.9\left(\frac{T}{|J|}\right)^{5/2}+O\left(\frac{T}{|J|}\right)^{3}\right\}$$

$$\chi=|J|^{-1}\left\{0.1667\left(\frac{|J|}{T}\right)^{2}+0.581\left(\frac{|J|}{T}\right)^{3/2}+0.68\left(\frac{|J|}{T}\right)^{1}+O\left(\frac{|J|}{T}\right)^{1/2}\right\}.$$

The first term of free energy coincides with the spin wave calculation. The first term of susceptibility coincides with Fisher's solution of classical Heisenberg Ferromagnet. We conclude $\alpha=-0.5$ and $\gamma=2$.

Takahashi-Yamada, Schlottmann 1985

Minoru Takahashi and Miki Yamada, J. Phys. Soc. Jpn. 54, 2808-2811 (1985) ‡

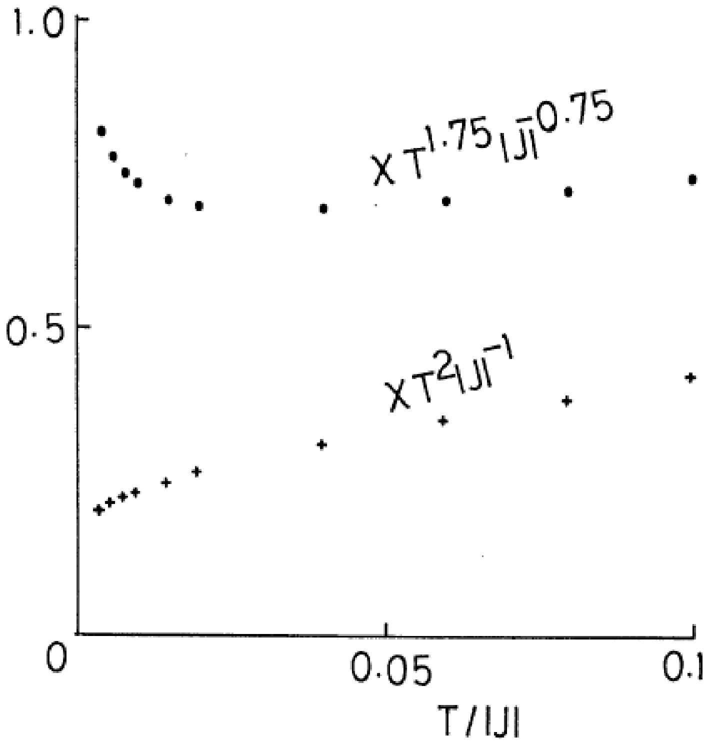


Fig. 1. $\chi T^{1.75}|J|^{-0.75}$ and $\chi T^2|J|^{-1}$ as a function of $T/|J|$. We find that $\gamma > 1.75$.

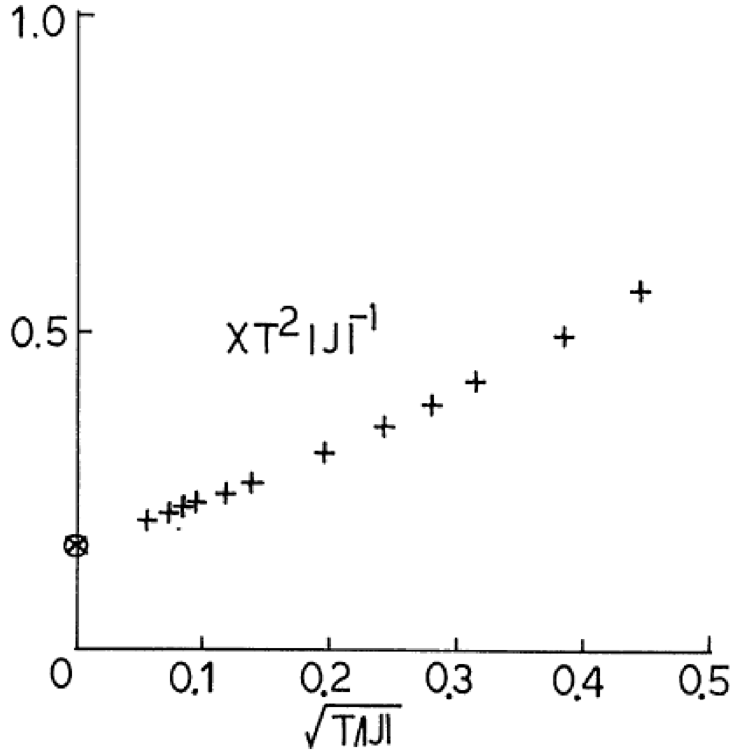


Fig. 2. $\chi T^2|J|^{-1}$ as a function of $\sqrt{T/|J|}$. In the limit $T \to 0$, it approaches to 0.167.

Minoru Takahashi and Miki Yamada, J. Phys. Soc. Jpn. 54, 2808-2811 (1985) ‡

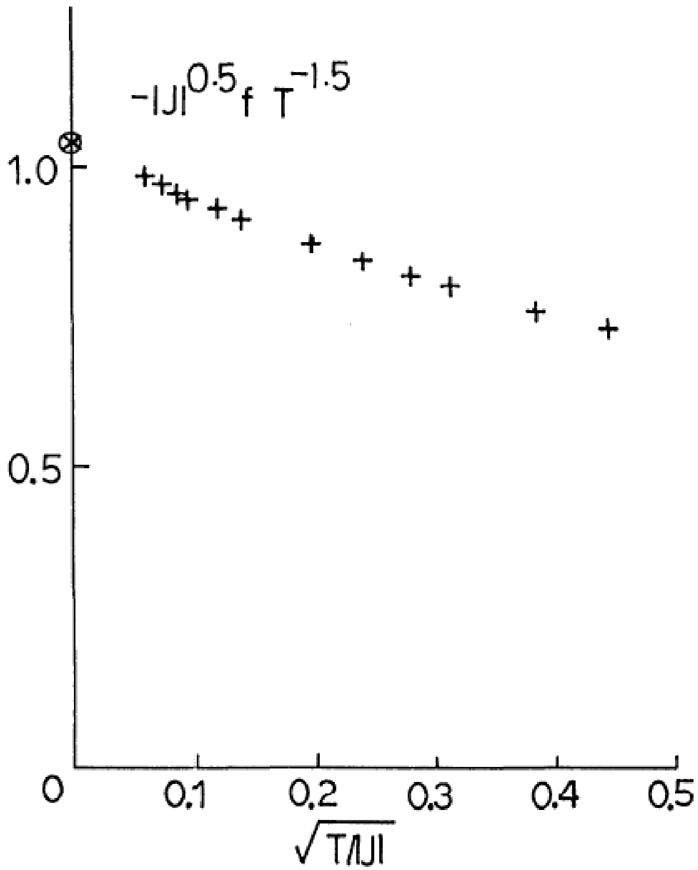


Fig. 3. $-fT^{-1.5}|J|^{0.5}$ as a function of $\sqrt{T/|J|}$. In the limit $T \to 0$, it approaches to 1.04.

References

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Nakamura, T. (1952) J. Phys. Soc. Jpn. **7**, 264.

Minoru Takahashi and Miki Yamada, J. Phys. Soc. Jpn. 54, 2808-2811 (1985) ‡

Modified spin-wave theory for ferromagnet

$$f = T[-1.042(T/J)^{1/2} + 1.00(T/J) - 0.9(T/J)^{3/2} + O(T^2)],$$

$$\chi = JT^{-2}[0.1667 + 0.581(T/J)^{1/2} + 0.68(T/J) + O(T^{3/2})].$$

In contrast, the usual spin-wave theory[6] gives

$$f = T[-1.042\,186\,9(T/J)^{1/2} - 0.066\,897\,1(T/J)^{3/2} - \cdots].$$

$$H = -J\sum_{\langle ij\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j - S^2) - 2h\sum_i^N S_i^z, \quad J > 0.$$

In 1D case MSW gives

$$f = T\left[\frac{\zeta(\frac{3}{2})}{(2\pi)^{1/2}}\left(\frac{T}{2SJ}\right)^{1/2} + \frac{T}{4S^2J} + \left(\frac{1}{2S^2}\frac{\zeta(\frac{1}{2})}{(2\pi)^{1/2}} - \frac{1}{8}\frac{\zeta(\frac{5}{2})}{(2\pi)}\right)\left(\frac{T}{2SJ}\right)^{3/2} + O(T^2)\right],$$

$$\chi = \tfrac{8}{3}S^4JT^{-2}\left[1 - \frac{3}{S}\frac{\zeta(\frac{1}{2})}{(2\pi)^{1/2}}\left(\frac{T}{2SJ}\right)^{1/2} + \frac{3}{S^2}\frac{\zeta^2(\frac{1}{2})}{2\pi}\frac{T}{2SJ} + O(T^{3/2})\right].$$

At $S = \frac{1}{2}$ these become

$$f = T[-1.042\,186\,9(T/J)^{1/2} + (T/J) - 1.232\,091\,9(T/J)^{3/2} + O(T^2)],$$

$$\chi = JT^{-2}[\tfrac{1}{6} + 0.582\,597\,4(T/J)^{1/2} + 0.678\,839\,6(T/J) + O(T^{3/2})].$$

Self consistent equation

$$w(x)=\frac{1}{N}\sum_{\boldsymbol{k}}\delta(x-\varepsilon(\boldsymbol{k}))\,. \qquad t\equiv T/(JS)\,, \qquad v\equiv-\mu/T\,.$$

$$S=\int_0^\infty\frac{w(x)dx}{\exp(xt^{-1}+v)-1}\,,$$

$$S'=S-\frac{1}{z}\int_0^\infty\frac{xw(x)dx}{\exp(xt^{-1}+v)-1}\,,$$

$$\frac{f}{T}=-vS+\int_0^\infty\ln(1-\exp(-xt^{-1}-v))w(x)dx-\frac{zJ}{2T}(S-S')^2\,,$$

$$\chi=\frac{4}{3T}\int_0^\infty\frac{\exp(xt^{-1}+v)w(x)dx}{(\exp(xt^{-1}+v)-1)^2}\,,$$

Bose-Einstein integral function:

$$F(\alpha,v)=\frac{1}{\Gamma(\alpha)}\int_0^\infty\frac{u^{\alpha-1}du}{e^{u+v}-1}=\frac{e^{-v}}{1^\alpha}+\frac{e^{-2v}}{2^\alpha}+\cdots\,. \qquad (3\cdot9)$$

Analytical property of this function near $v=0$ is known.[13] If α is not a positive integer we have

$$F(\alpha,v)=\Gamma(1-\alpha)v^{\alpha-1}+\sum_{n=0}^{\infty}(n!)^{-1}(-v)^n\zeta(\alpha-n)\,. \qquad (3\cdot10)$$

When α is a positive integer, we have

$$F(\alpha,v)=(-v)^{\alpha-1}((\alpha-1)!)^{-1}\left\{\sum_{r=1}^{\alpha-1}\frac{1}{r}-\ln v\right\}+\sum_{n\neq\alpha-1}(n!)^{-1}(-v)^n\zeta(\alpha-n)\,. \qquad (3\cdot11)$$

Schlottmann's low-temerature susceptibility

$$\chi = 0.84 J T^{-2}\left[\frac{1}{\ln(J/T)} + \frac{\ln\ln(J/T)}{\ln^2(J/T)}\right].$$

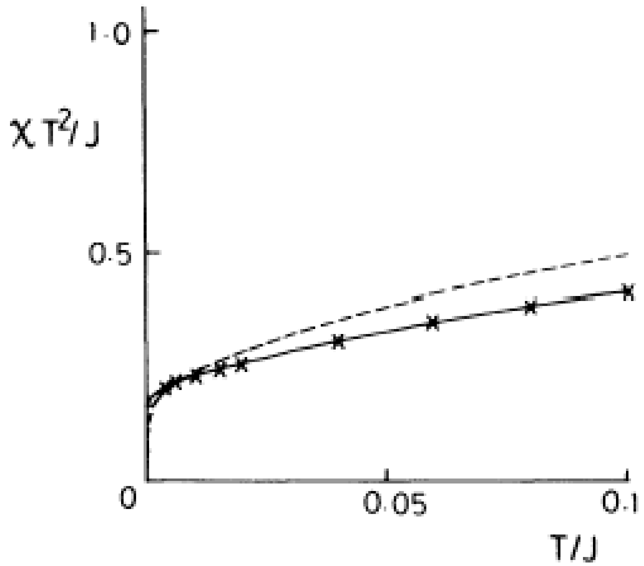


FIG. 1. $\chi T^2 J^{-1}$ as a function of TJ^{-1} for the $S=\frac{1}{2}$ Heisenberg linear chain. Crosses are results of the Bethe-*Ansatz* integral equation from Ref. 2. Solid line is my expansion (18). Dashed line is Schlottmann's susceptibility (19) taken from Ref. 4. My expansion formula coincides accurately with numerical results of the Bethe-*Ansatz* integral equation.

2D square lattice system and classical system

$$f = -(4\pi JS)^{-1} T^2 \{\zeta(2) + \tfrac{1}{8}\zeta(3)(T/JS) + O(T^2)\}, \quad (20)$$

$$\chi = (3\pi JS)^{-1} \exp(4\pi JS^2/T)[1 + O(T)]. \quad (21)$$

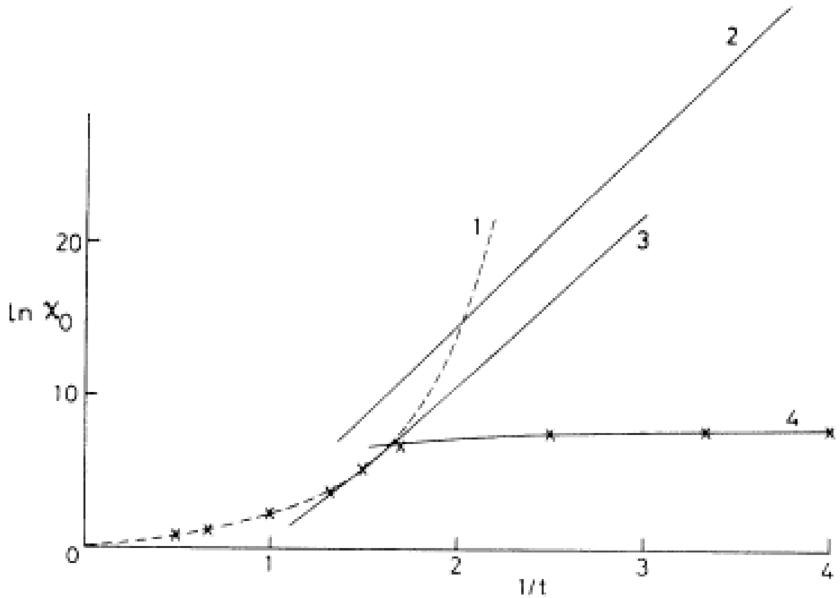


FIG. 3. Logarithm of susceptibility as a function of $1/t$. Line 1 is the result of high-temperature expansion (3.16). Line 2 shows the spin-wave results for an infinite system (1.4). Line 3 is the result of the Shenker-Tobochnik formula (1.7). Line 4 shows the spin-wave results for the 64×64 lattice. Crosses are the Monte Carlo results for the 64×64 lattice.

Modified spin-wave theory for square lattice antiferromagnet

Phys. Rev. B40 2494 (1989),Arovas-Auerbach, Hirsch-Tang,

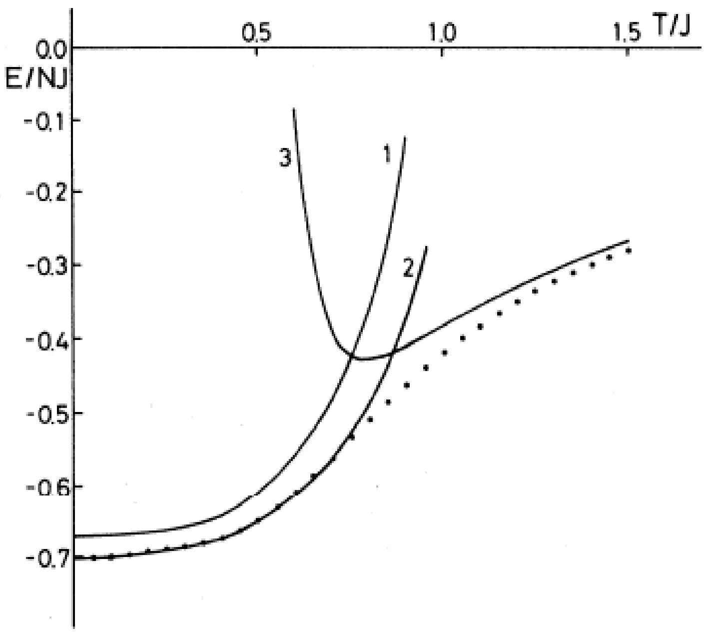


FIG. 1. Energy per site calculated by spin-wave theory for 4×4 and 64×64 lattices. Small circles are results of exact diagonalization of the 4×4 lattice. Agreement is very good in the region $0 \le T \le 0.7J$. Line 1, spin-wave result of the 64×64 lattice; line 2, spin-wave result of the 4×4 lattice; and line 3, high-temperature expansion.

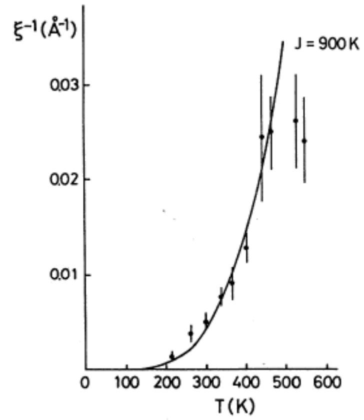


FIG. 3. Inverse of correlation length. Dots with error bars are results of neutron experiment of La_2CuO_4 taken from Ref. 3. The solid line is Eq. (27a) at $J = 900$ K.

$$S+\frac{1}{2}=\frac{1}{2}\int_0^1(1-\eta^2x^2)^{-1/2}\coth\left[\frac{\lambda}{2T}(1-\eta^2x^2)^{1/2}\right]w(x)dx\ ,$$

$$\left[S+\frac{1}{2}\right]-\frac{\lambda\eta^2}{4J}=\frac{1}{2}\int_0^1(1-\eta^2x^2)^{1/2}\coth\left[\frac{\lambda}{2T}(1-\eta^2x^2)^{1/2}\right]w(x)dx\ .$$

At $\sqrt{1-\eta}\ll T/\lambda\ll 1$ these are as follows:

$$S+\frac{1}{2}=w(1)\frac{T}{\lambda}\left[\frac{1}{2\eta}\ln\left[\frac{1+\eta}{1-\eta}\right]-\ln\left[\frac{2\lambda}{T}\right]\right]+\frac{1}{2}\int_0^1(1-x^2)^{-1/2}w(x)dx+O(T^3)\ ,$$

$$\left[S+\frac{1}{2}\right]-\frac{\lambda\eta^2}{4J}=\frac{1}{2}\int_0^1(1-x^2)^{1/2}w(x)dx+2w(1)\zeta(3)\left[\frac{T}{\lambda}\right]^3+O(T^5)\ .$$

$$\xi\equiv[8(\eta^{-2}-1)]^{-1/2}$$
$$=\frac{\sqrt{2}Jm_1}{T}\exp\left[\frac{2\pi Jm_0m_1}{T}\right][1+O(T^2)]\ .$$

$$m_0\equiv S+\tfrac{1}{2}-\tfrac{1}{2}\int_0^1(1-x^2)^{-1/2}w(x)ds$$
$$=S-0.196\,60\ . \qquad (18)$$

$$m_1\equiv S+\tfrac{1}{2}-\tfrac{1}{2}\int_0^1(1-x^2)^{1/2}w(x)dx$$
$$=S+0.078\,974\ .$$

Quantum Monte Carlo

1. Formulation of path integral Monte Carlo method
2. Application to He4 and 2D electron gas
3. Elementary excitation and correlation function of Haldane chain

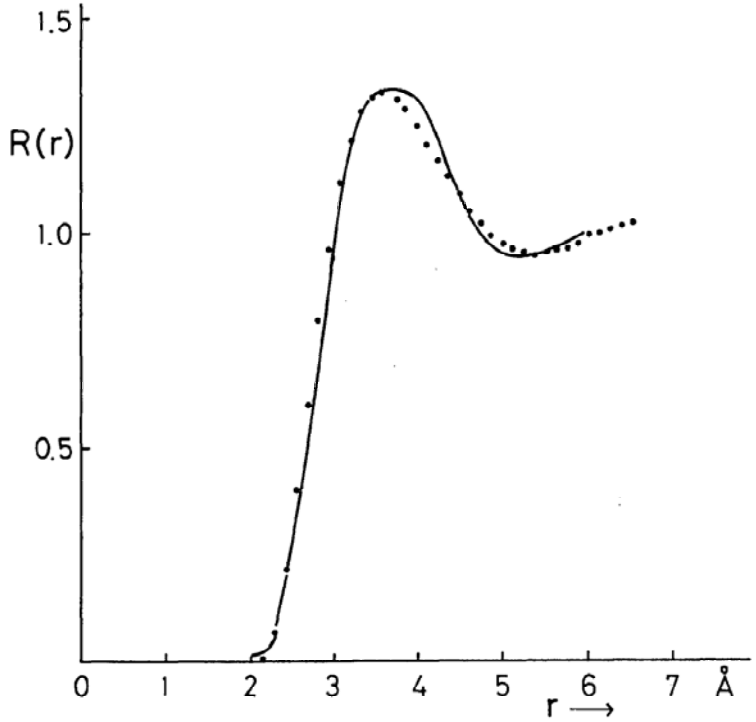


Fig. 3. Radial distribution function at $T=5.04$ K and $d=0.02375$ mol/cm^3. The dots are results of our path-integral Monte Carlo calculation. The solid line is the experimental result from Fig. 4 of ref. 14.

Minoru Takahashi and Masatoshi Imada,
J. Phys. Soc. Jpn. 53, 3871-3877 (1984) ‡

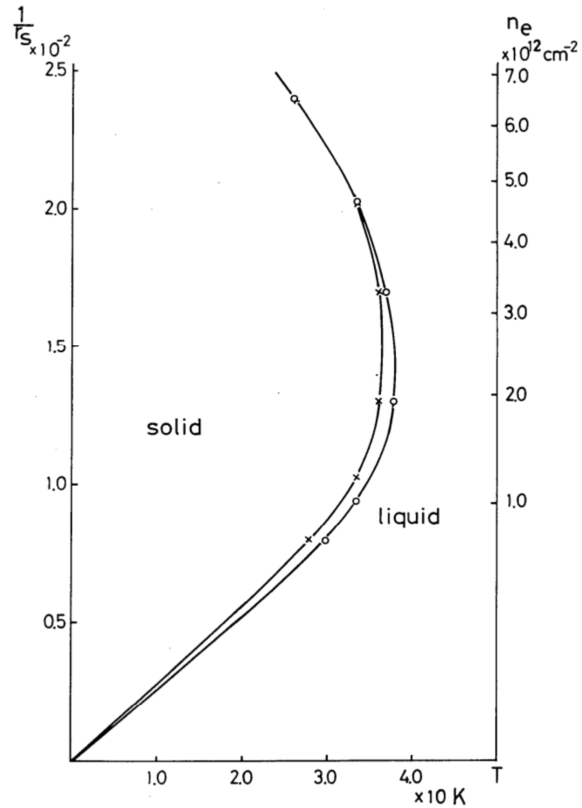


Fig. 5. Phase diagram for 12 electrons system. The curves show the melting transition. Two curves are obtained from the hysteresis.

Masatoshi Imada and Minoru Takahashi,
J. Phys. Soc. Jpn. 53, 3770-3781 (1984) ‡

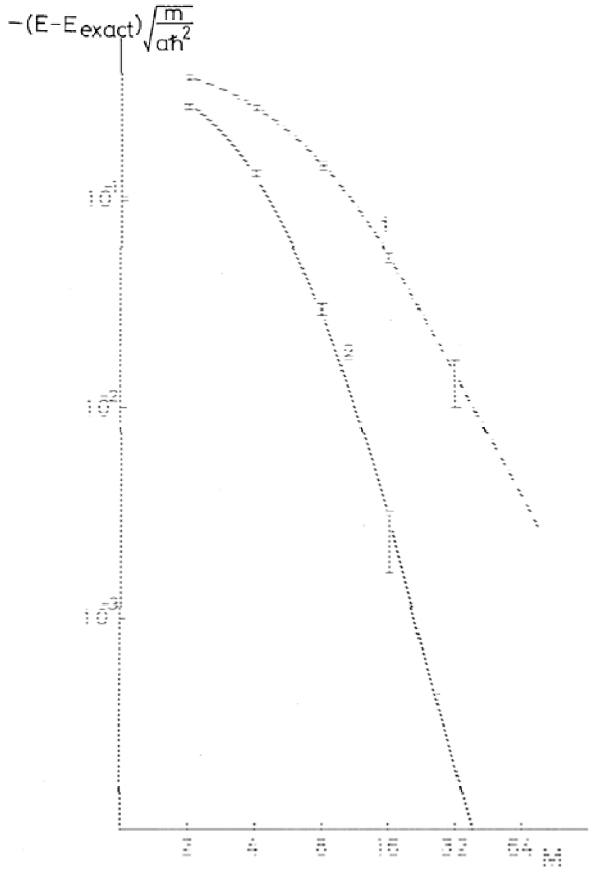


Fig. 1. Deviations of Monte Carlo results from the exact value (22) as a function of M for the total energy of one-dimensional harmonic oscillator at the temperature $\beta^{-1}=0.0625\hbar\sqrt{a/m}$. Series 1 is the result of previous paper and series 2 is that of this paper. Error bars illustrate the results of 20000 steps of Monte Carlo calculation. Dashed and solid lines are exact deviations of these methods obtained from eqs. (22), (25) and (26).

$$H = H_0 + H_1,$$

$$H_0 = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\frac{\partial^2}{\partial \boldsymbol{r}_i^2}, \quad H_1 = V(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_N).$$

$$e^{-\beta(H_0+H_1)} = \lim_{M\to\infty}\left(e^{-(\beta H_0/M)}e^{-(\beta H_1/M)}\right)^M.$$

$$\mathrm{Tr}\exp\{-\beta(H_0+H_1)\} = \mathrm{Tr}\,[\exp\{(-\beta/M)H_0\}\exp\{(-\beta/M)H_1'\}]^M + O(\beta^5 M^{-4}),$$

$$H_1' = H_1 + \frac{1}{24}\left(\frac{\beta}{M}\right)^2[H_1, [H_0, H_1]].$$

In the problem of Hamiltonian (1) we have

$$H_1' = V' = V(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_N) + \frac{1}{24}\frac{\hbar^2}{m}\left(\frac{\beta}{M}\right)^2\sum_{i=1}^{N}\left(\frac{\partial V}{\partial \boldsymbol{r}_i}\right)^2.$$

Minoru Takahashi and Masatoshi Imada, J. Phys. Soc. Jpn. 53, 3765-3769 (1984) ‡

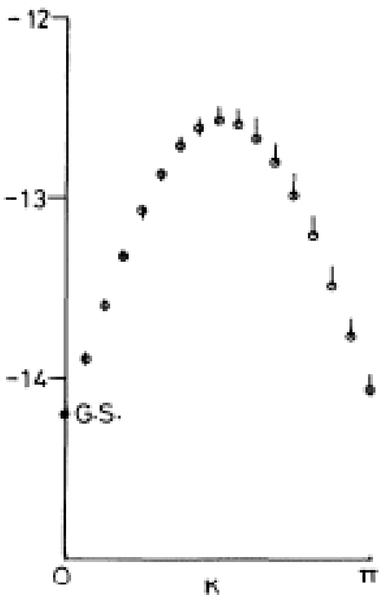


FIG. 2. $E_1(K)/J$ for $N=32$, $S=\frac{1}{2}$ HAC. Circles are results of the Bethe-*Anstaz* equation (Ref. 8). Bars are results of the MC calculation. Length of the bar represents error of MC calculation.

Seishi Takagi, Hiroyuki Deguchi, Kazuyoshi Takeda, Masaki Mito and Minoru,
J. Phys. Soc. Jpn. 65, 1934-1937 (1996) ‡

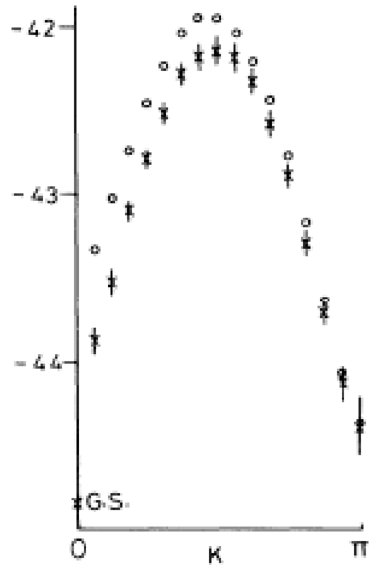


FIG. 3. $E_1(K)/J$ for $N=32$, $S=1$ HAC. The spectrum has a gap at $K=\pi$. The value of the gap is about $0.4J$ and coincides with NB's calculation. Small circles are the upper bound of $E_1(K)/J$ given in Ref. 10. This upper bound was calculated from the structure factor and variational relation.

Logarithmic anomaly of anti-ferromagnetic chain

熱学・統計力学 p.123 裳華房　久保亮五 ‡

[26] 熱力学第3法則によれば，エントロピー S は，$T \to 0$ において磁場 H によらない極限値をもつ．したがって $(\partial S/\partial H)_T \to 0$ $(T \to 0)$．問題 [24] の (2) により，$\lim_{T \to 0} (\partial M/\partial T)_H = 0$，ここに　$M = \chi_T H$　を入れると

$$\lim_{T \to 0} (\partial \chi_T / \partial T) = 0.$$

(注) ゆえに，Curie の法則 $\chi = C/T$，Curie-Weiss の法則 $\chi = C/(T+\theta)$ はいずれも，有限なある温度までしか成り立たない．$T \to 0$ では必らずこれらの法則からの外れが起こる．

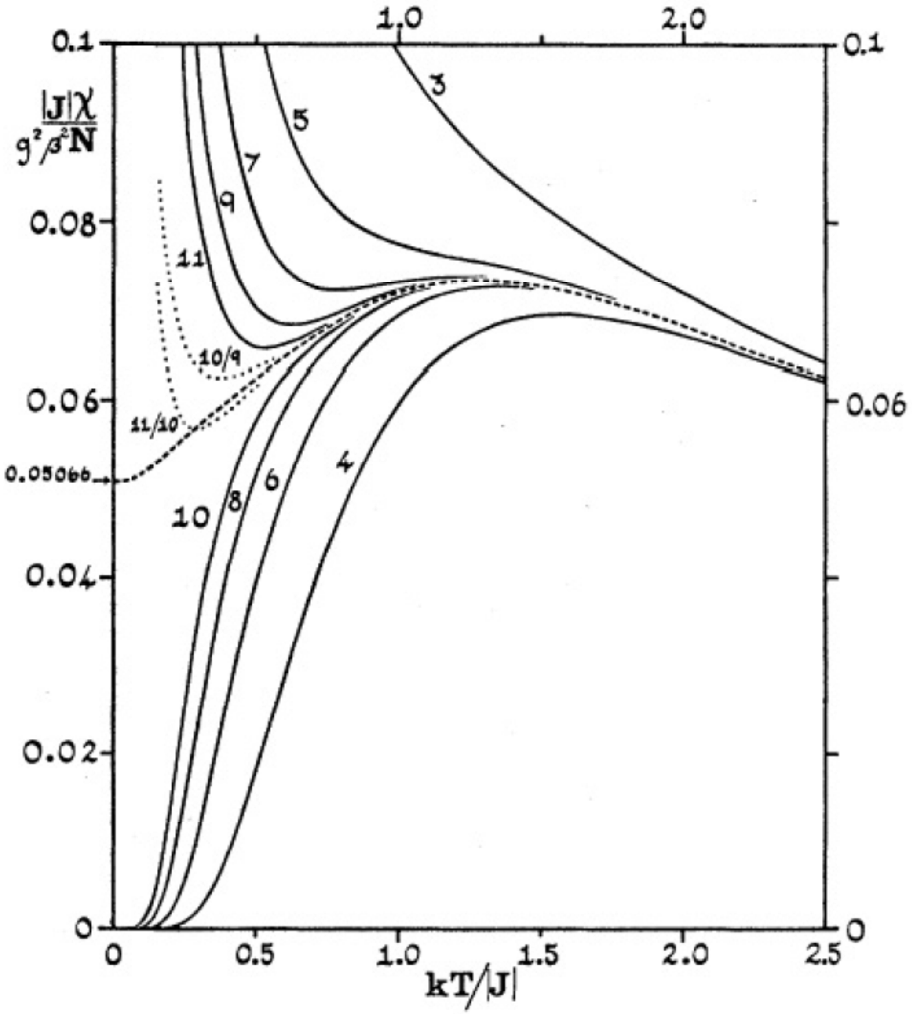


FIG. 14. Antiferromagnetic susceptibility versus temperature for finite Heisenberg rings (solid curves) and the estimated limit for infinite rings (dashed curve). The dotted curves are means of $N=9$ and 10, and $N=10$ and 11 weighted as in (a) and (c) (Ref. 35), respectively.

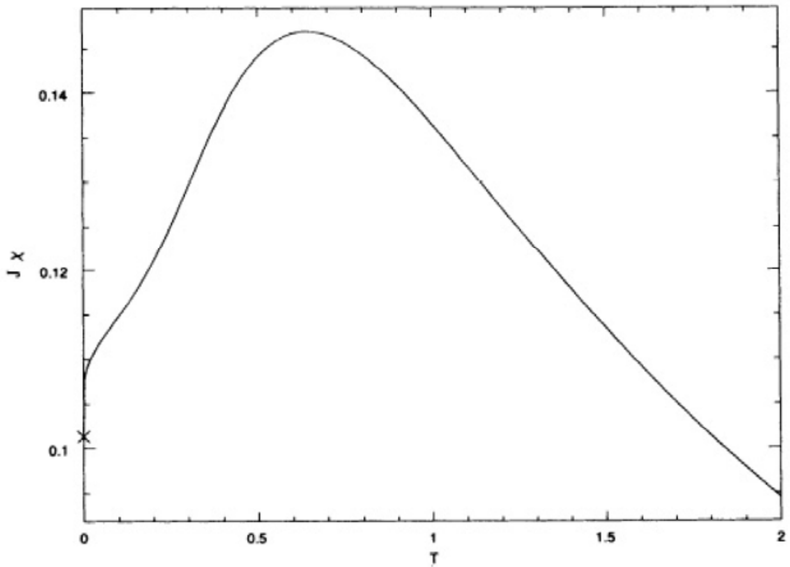


FIG. 1. $\chi(T)$ from the Bethe ansatz. $\chi(0)$ is taken from Ref. [2].

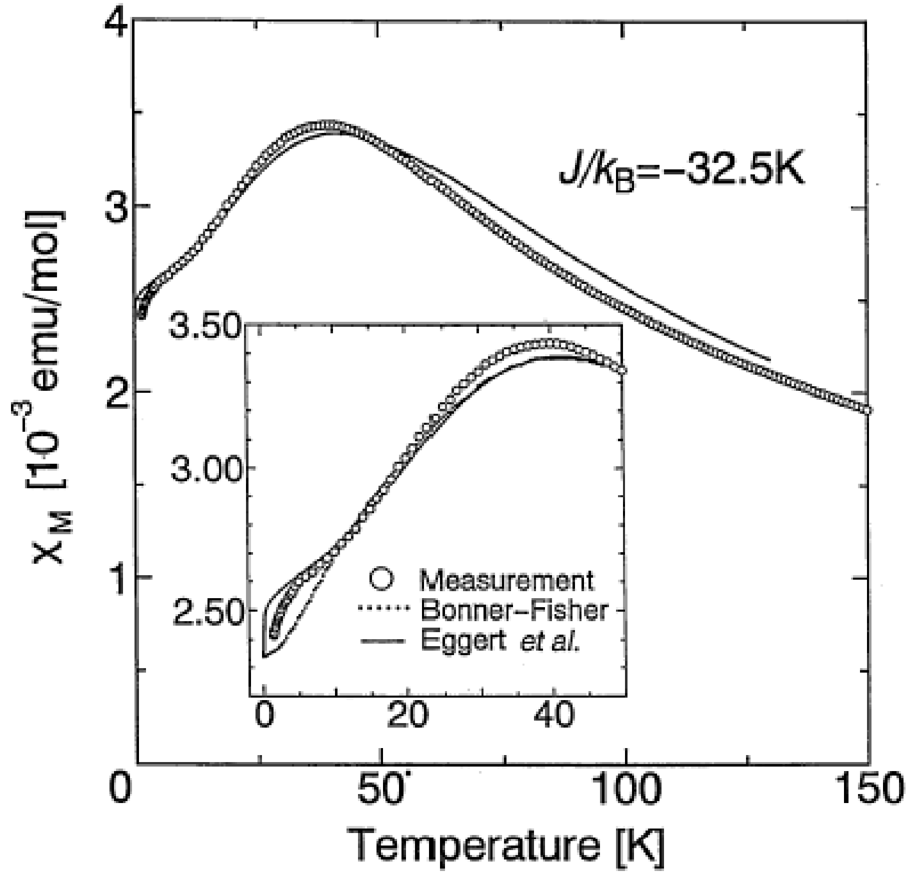
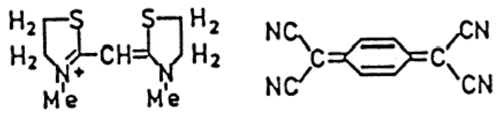


Fig. 3. Temperature dependence of the paramagnetic susceptibility of the salt. The low temperature region of the susceptibility is enlarged and inset in the figure. The dotted line is the curve obtained by Bonner and Fisher, whereas the solid line is the curve obtained by Eggert *et al.*



(a)DMTzNC$^+$ (b) TCNQ

Seishi Takagi, Hiroyuki Deguchi, Kazuyoshi Takeda, Masaki Mito, and Minoru Takahashi, J. Phys. Soc. Jpn. 65, 1934-1937 (1996) ‡

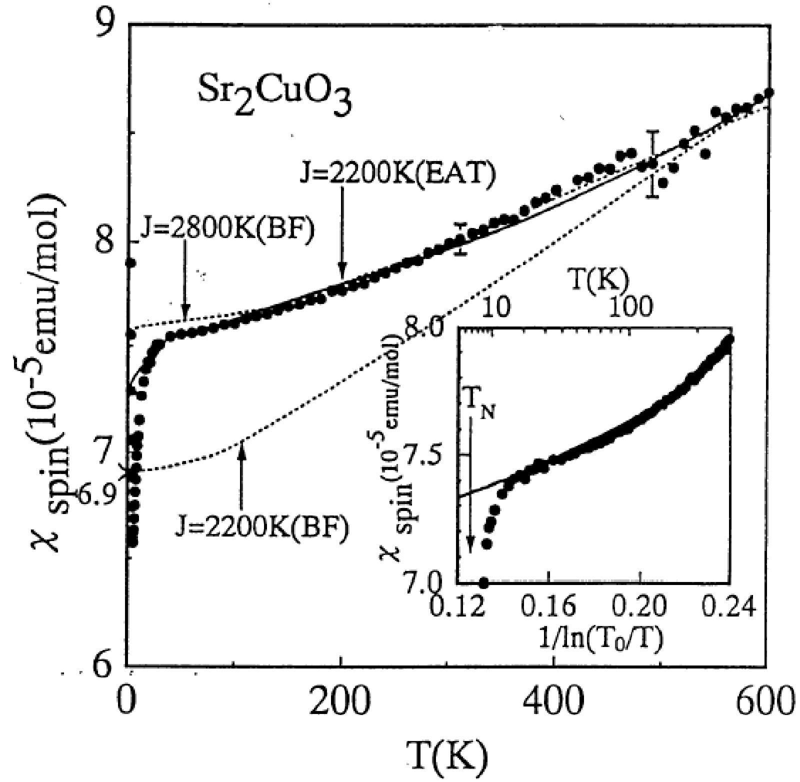


FIG. 4. $\chi_{\rm spin}$ for Sr_2CuO_3 compared to theoretical calculations by EAT [3] with $J = 2200$ K (solid line) and by BF with $J = 2200$ and 2800 K (dotted line) in the temperature range below 600 K. The cross (×) at $T = 0$ K indicates the theoretical susceptibility at $T = 0$ K for $J = 2200$ K. Inset: the experimental (dot) and theoretical (line) $\chi_{\rm spin}$ as a function of $[\ln(T_0/T)]^{-1}$.

Four-spin interaction term

$$H = \sum t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + I \sum n_{i\uparrow} n_{i\downarrow} .$$

$$H = H_0 + \lambda V$$

$$h = \lambda^2 h_2 + \lambda^4 h_4 + O(\lambda^6)$$

$$h_2 = I^{-1} \sum_{i<j} t_{ij}^2 (\sigma_i \sigma_j - 1),$$

$$h_4 = I^{-3} \Big[\sum_{i<j} 4 t_{ij}^4 (1 - \sigma_i \sigma_j) + \sum_{i \neq k} t_{ij}^2 t_{jk}^2 (\sigma_i \sigma_k - 1) + \sum_{\substack{i<j<l,\, i<k \\ k \neq j,l}} t_{ij} t_{jk} t_{kl} t_{li} \big(5(\sigma_j \sigma_k)(\sigma_i \sigma_l)$$
$$+ 5(\sigma_i \sigma_j)(\sigma_k \sigma_l) - 5(\sigma_i \sigma_k)(\sigma_j \sigma_l) - \sigma_i \sigma_j - \sigma_j \sigma_k - \sigma_k \sigma_l - \sigma_l \sigma_i$$
$$- \sigma_i \sigma_k - \sigma_j \sigma_l + 1\big) \Big]$$

M. Takahashi, J. Phys. C: Solid State Phys. 10, 1289-7301 (1977) ‡

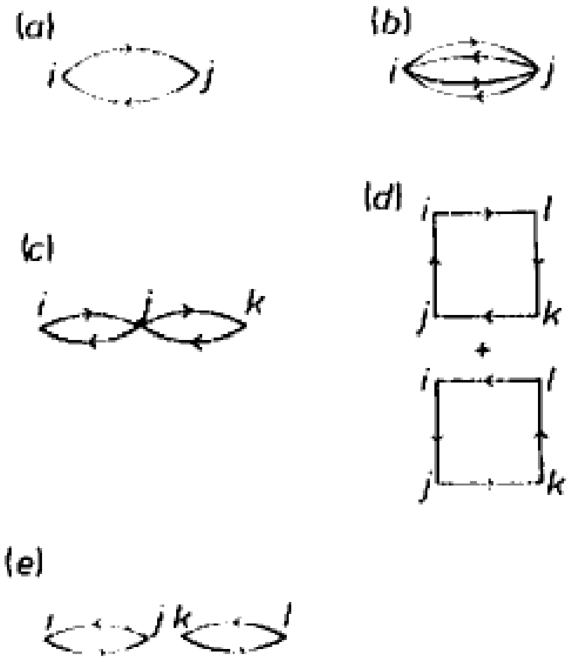


Figure 1. In terms of the diagrams, the t_{ij}^2 term in h_2 corresponds to (*a*); t_{ij}^4, $t_{ij}^2 t_{jk}^2$ and $t_{ij} t_{jk} t_{kl} t_{li}$ in h_4 corresponds to (*b*), (*c*), and (*d*), respectively. Unlinked diagrams such as (*e*) disappear.

$$\langle \sigma_i \sigma_{i+1} \rangle_0 = 1 - 4 \ln 2 = -1{\cdot}772\,588\,72$$

$$\langle \sigma_i \sigma_{i+2} \rangle_0 = 1 - 16 \ln 2 + 9\zeta(3) = 0{\cdot}728\,157\,2394.$$

M. Takahashi, J. Phys. C: Solid State Phys. 10, 1289-7301 (1977) ‡

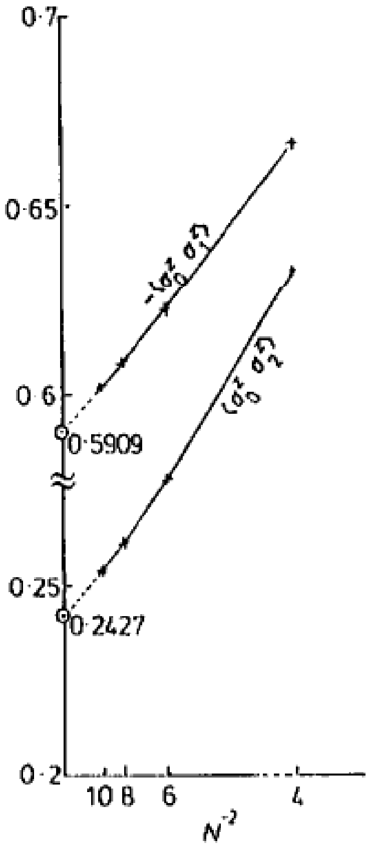


Figure 2. The first- and second-neighbour correlation functions of an antiferromagnetic ring with N atoms are plotted as functions of $1/N^2$. In the limit $N = \infty$, these values approach the theoretical values. Table 2 of Bonner and Fisher (1964) was used.

M. Takahashi, J. Phys. C: Solid State Phys. 10, 1289-7301 (1977) ‡

有機強磁性体の研究

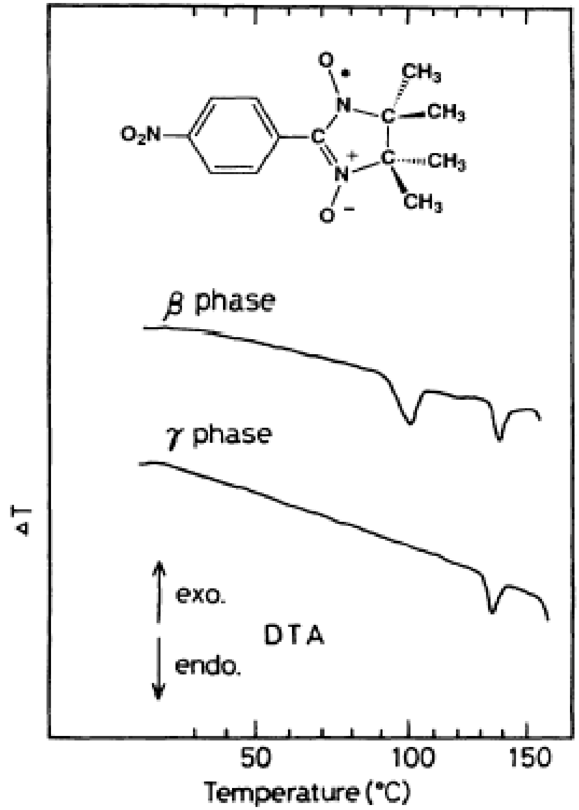


FIG. 1. DTA curves of *β*- and *γ*-phase samples heated at 3 °C/min in air and the molecule of *p*-NPNN.

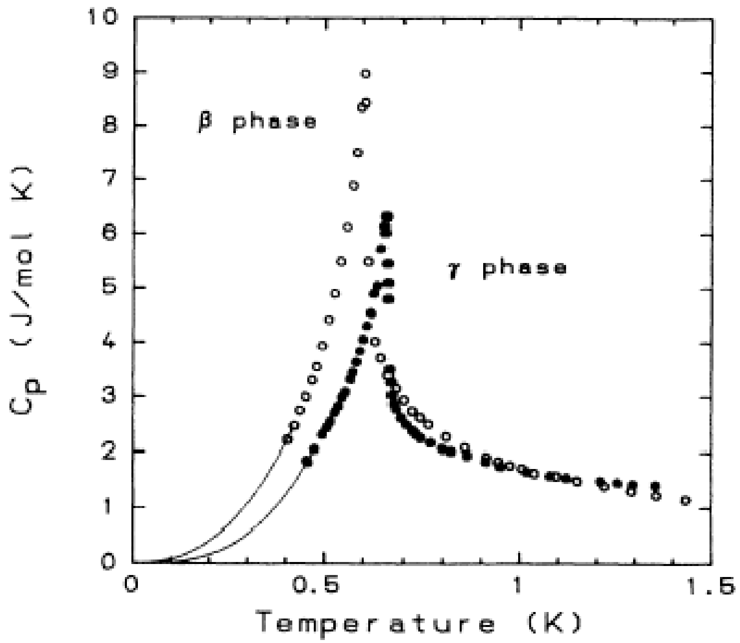
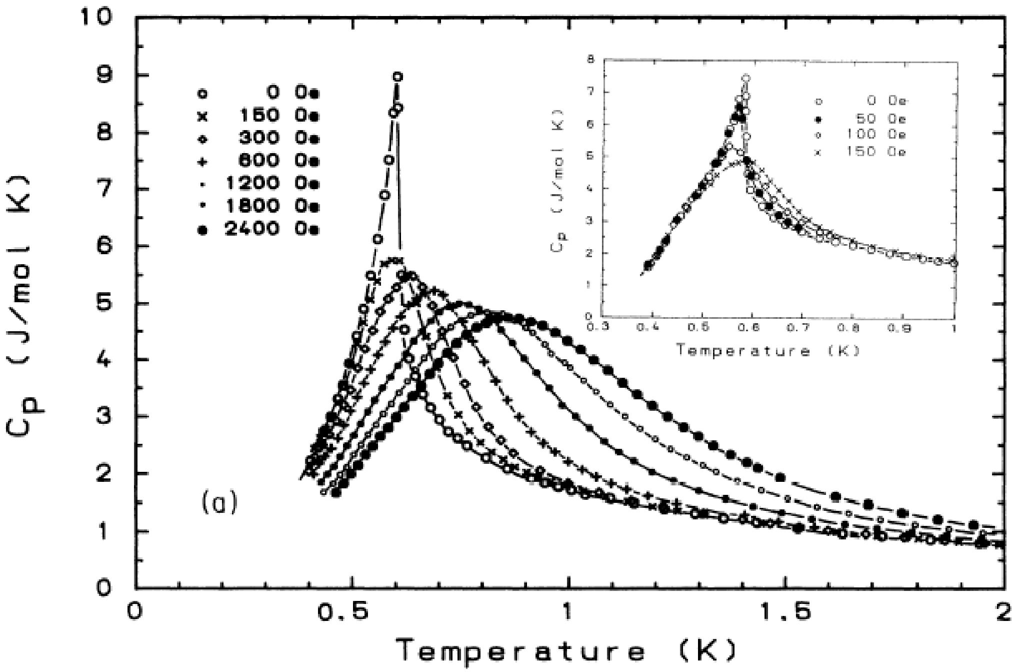


FIG. 3. Zero-field specific-heat curves of *γ*- and *β*-phase samples. The smooth curves at the low-temperature end represent the spin-wave approxmation for three-dimensional antiferromagnetic and ferromagnetic systems (see text).



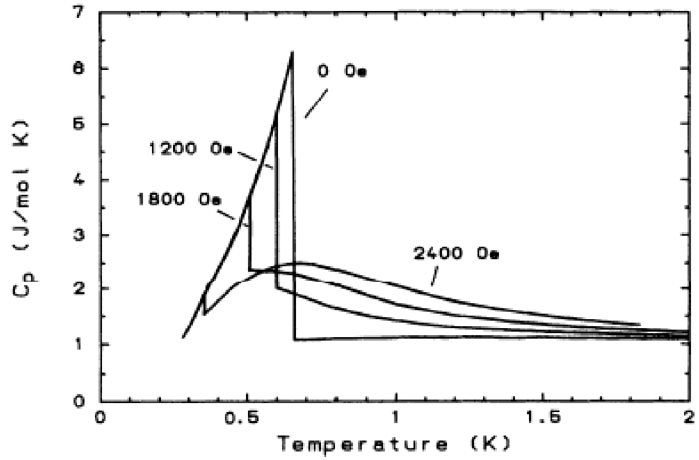
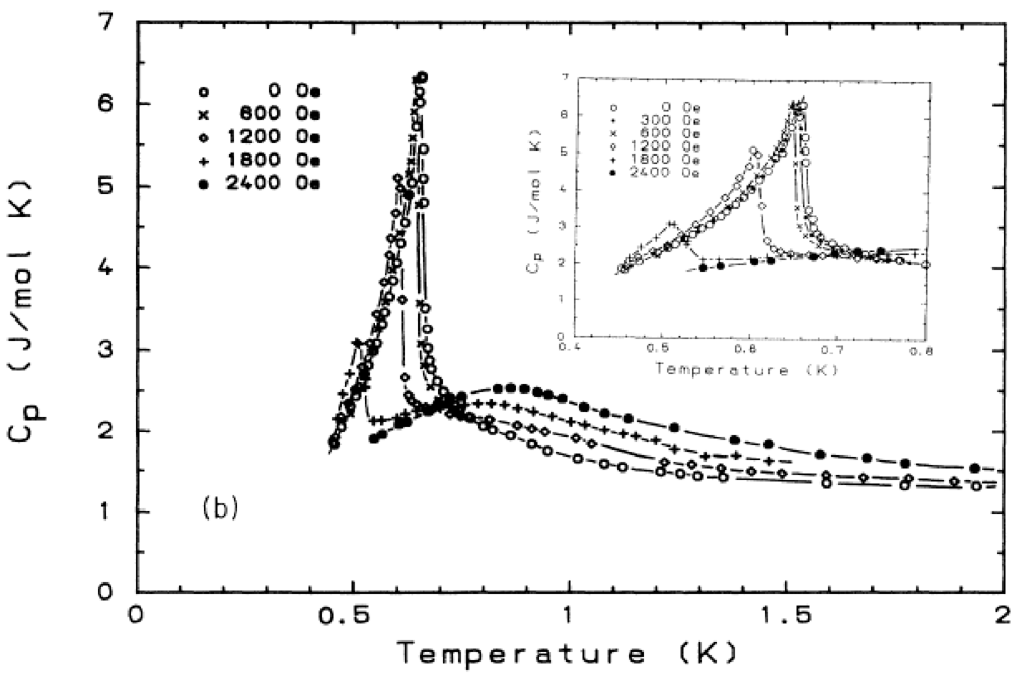
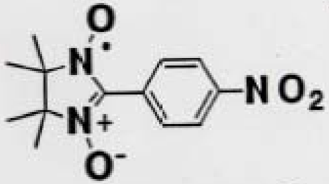


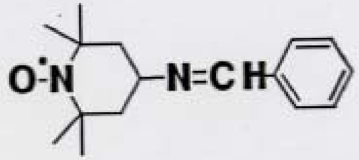
FIG. 13. Theoretical magnetic specific heat of a quasi-one-dimensional Heisenberg ferromagnet with $J = 4.3$ K, $J' = 0.224$ K, and $J'' = -0.176$ K. The interchain couplings were determined by the mean-field approximation.



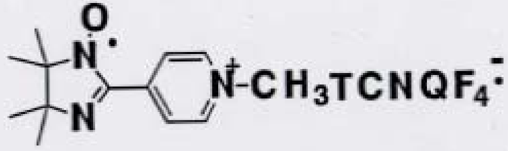
Organic Ferromagnets



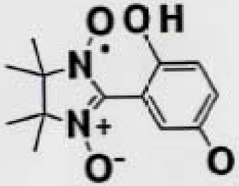
$T_c = 0.6$ K



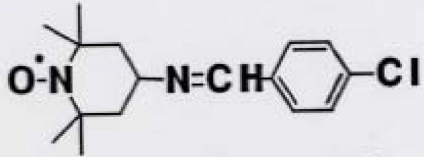
$T_c = 0.18$ K



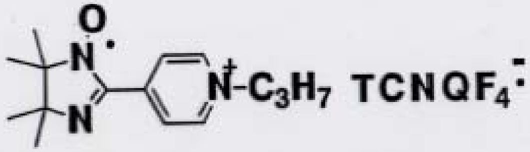
$T_c = 0.45$ K



$T_c = 0.5$ K

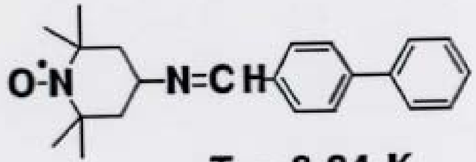


$T_c = 0.4$ K

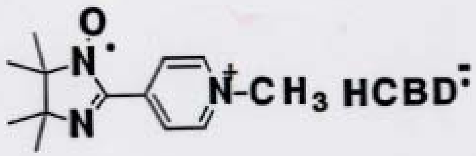


$T_c = 0.6$ K

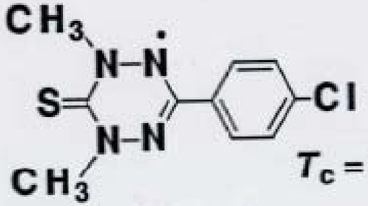
$T_c = 1.48$ K



$T_c = 0.24$ K

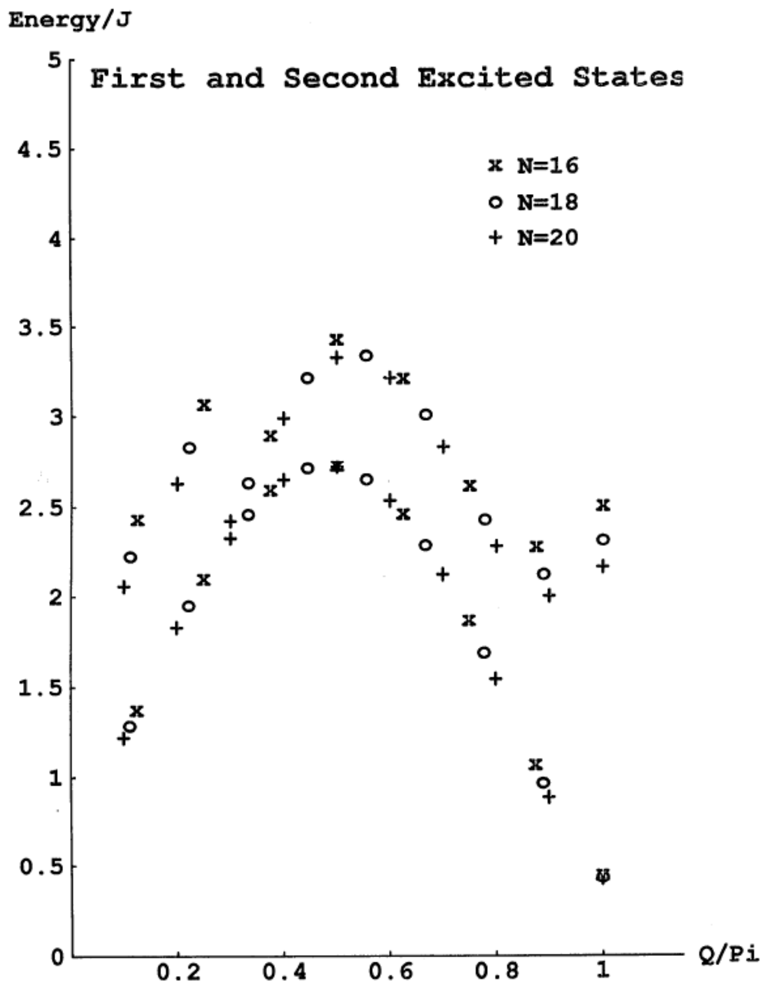


$T_c = 0.5$ K



$T_c = 0.7$ K

Haldane chain



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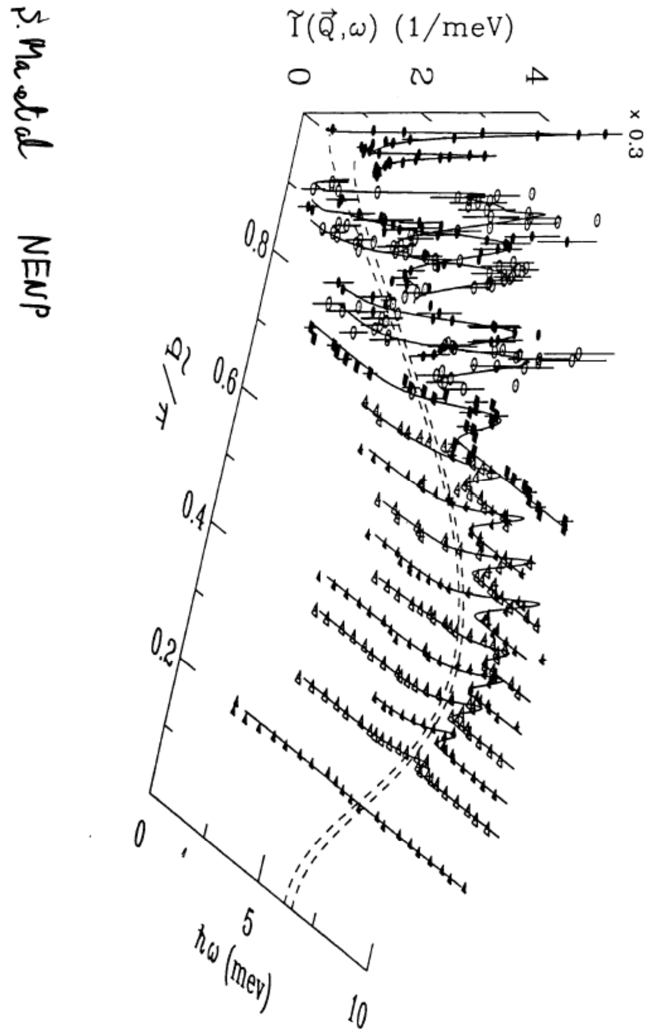

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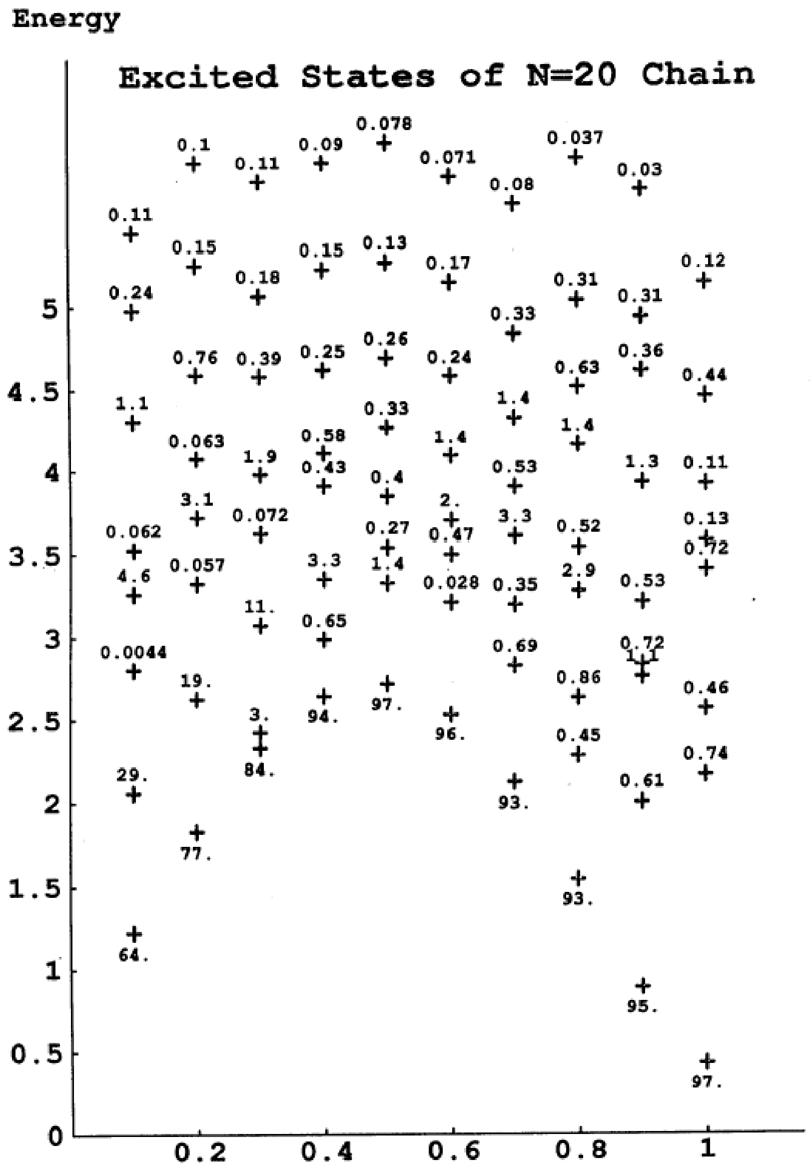

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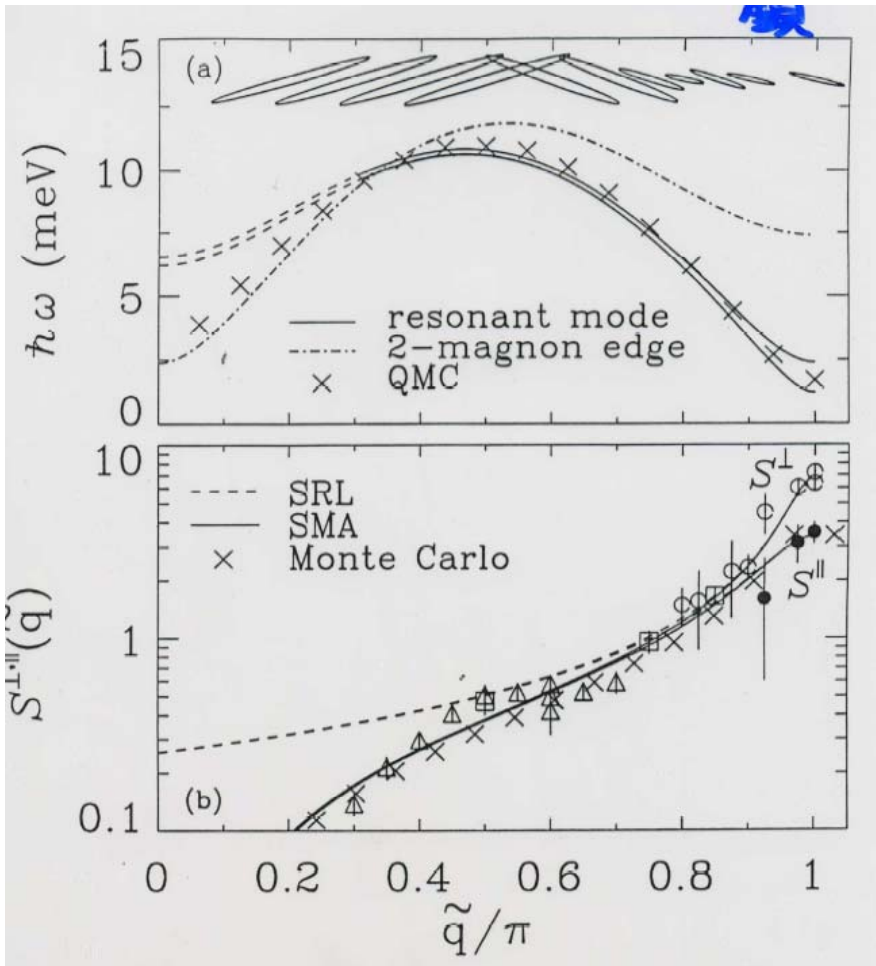

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After 2000

1. New simplified form of TBA equations

This equation is convenient to get the high temperature expansion of thermodynamic quantities.XXZ chain and Perk-Schultz model.

2. High-temperature expansion of Hubbard model and TBA equations

3. Calculation of correlation functions of XXX and XXZ chain

New simplified form of TBA equations

$$\mathcal{H}(J,\Delta,h) = -J\sum_{l=1} S_l^x S_{l+1}^x + S_l^y S_{l+1}^y + \Delta(S_l^z S_{l+1}^z - \frac{1}{4}) - 2h\sum_{l=1} S_l^z,$$

$$h \geq 0, \tag{1}$$

thermodynamic Bethe ansatz equation at temperature T is

$$\ln\eta_1(x) = \frac{2\pi J\sinh\phi}{T\phi}\mathrm{s}(x) + \mathrm{s} * \ln(1+\eta_2(x)),$$

$$\ln\eta_j(x) = \mathrm{s} * \ln(1+\eta_{j-1}(x))(1+\eta_{j+1}(x)), \quad j = 2,3,...,$$

$$\lim_{l\to\infty}\frac{\ln\eta_l}{l} = \frac{2h}{T}. \tag{2}$$

Here we put

$$\Delta = \cosh\phi,\ Q \equiv \pi/\phi,\ \mathrm{s}(x) = \frac{1}{4}\sum_{n=-\infty}^{\infty}\mathrm{sech}\Big(\frac{\pi(x-2nQ)}{2}\Big),$$

$$\mathrm{s} * f(x) \equiv \int_{-Q}^{Q}\mathrm{s}(x-y)f(y)\mathrm{d}y. \tag{3}$$

The free energy per site is

$$f = \frac{2\pi J\sinh\phi}{\phi}\int_{-Q}^{Q}\mathrm{a}_1(x)\mathrm{s}(x)\mathrm{d}x - T\int_{-Q}^{Q}\mathrm{s}(x)\ln(1+\eta_1(x))\mathrm{d}x,$$

$$\mathbf{a}_1(x) \equiv \frac{\phi \sinh \phi/(2\pi)}{\cosh \phi - \cos(\phi x)}. \tag{4}$$

On the contrary new equation is

$$u(x) = 2\cosh(\frac{h}{T}) + \oint_C \frac{\phi}{2}\Big(\cot \frac{\phi}{2}[x - y - 2i] \exp[-\frac{2\pi J \sinh \phi}{T\phi}\mathbf{a}_1(y+i)]$$

$$+ \cot \frac{\phi}{2}[x - y + 2i] \exp[-\frac{2\pi J \sinh \phi}{T\phi}\mathbf{a}_1(y-i)]\Big) \frac{1}{u(y)} \frac{\mathrm{d}y}{2\pi i}, \tag{5}$$

and free energy is given by

$$f = -T \ln u(0). \tag{6}$$

$$u(x) = \exp[\textstyle\sum_{n=0}^{\infty} a_n(x)(\tilde{J}/T)^n]$$

TABLE I. Series coefficients α_n for the high-temperature expansion of the specific heat $C = \sum_n \frac{\alpha_n}{n!}(\frac{J}{4T})^n$ at $h = 0$.

n	α_n	n	α_n
0	0	26	484455914465376683487755420408217600
1	0	27	−1592964364128699671723658807556964352
2	6	28	−16592223413777236744548930659363711 87712
3	−36	29	53827694891210973745020673240061454581760
4	−360	30	5090517962961447184851808942927438864711680
5	7200	31	−388446833192725659973817494776649147157053440
6	15120	32	−11028658525378274359384407389662010654796546048
7	−1848672	33	2255854109806569120380670028755308714386167693312
8	11426688	34	−18878702580622989070078793482363993425701807063040
9	594846720	35	−11721570087037734701356860480896473609272542720163840
10	−11558004480	36	527183038642469386328859769728396518893185382125404160
11	−199812856320	37	52548749252010967993948480669499712309299856992951599104
12	10106191180800	38	−5382365237582398925074954773487741035075672601159589167104
13	19376365252608	39	−150281021589219619860159284209265140804955107276364175114240
14	−9289795522775040	40	44482678475307391762958213932359681737961800852665438128046080
15	121944211136778240	41	−670778300712303276022754187872671936481343744506621812675706880
16	8791781390116945920	42	−323311185126253530334911142992092649497388429937499549362387156992
17	−310402124957945954304	43	19271391500067613736198673193545354611765664770995927250862568636416
18	−7225535925744106143744	44	1963797073102024140530884388201619017857423297479642613447074848440320
19	643407197363813620776960	45	−261757449501391383349154989821467694962901907072496780634929173522022400
20	96147483542540314214400	46	−6715036186134671522475926929150627328836680429076585020863949295740518400
21	−1279121513829538179364945920	47	2897640509780835688484069216581936412870887902144153768250804439297575354368
22	27962069861743501862336200704	48	−67884583842448252705729493380589916284543590592089243545625816663055684075520
23	2398518627113966015427501883392	49	−27839667354545349510646207322267839343449407617219100508752156300912706663219200
24	−129834725539335848980192847462400	50	2130333568970965233678580974509426707048585535358286474483865352948915543579033600
25	−3493877000064415911285457158144000	51	216827879657653769500650387534438914339017251205042192428944424756474567924803174400

High temperature expansion of Hubbard model

[7] I.C. Charret, E.V. Corrêa Silva, S.M. de Souza, O. Rojas Santos, M.T. Thomaz, and A.T. Costa, Jr., Phys. Rev. B 64, 195127 (2001).

U=4

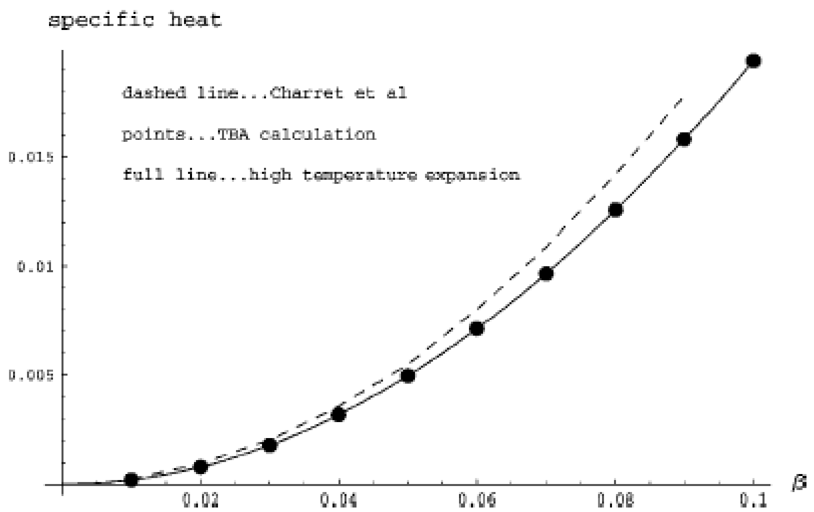

FIG. 1. Specific heat at $U=4$, $h=0$, and $U/2-A=0$. Points are our results of TBA calculations and the dashed line is the calculation of Charret *et al.* The solid line is the high-temperature expansion.

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