Spin-wave stiffness of the Heisenberg antiferromagnet at zero temperature

C. J. Hamer,* Zheng Weihong,† and J. Oitmaa‡
School of Physics, The University of New South Wales, Sydney, NSW 2052, Australia
(Received 12 April 1994; revised manuscript received 19 May 1994)

The spin-wave stiffness ρ_s of the Heisenberg antiferromagnet at zero temperature is calculated in two ways, by spin-wave theory and by series expansion about the Ising limit, extending previous results. The two methods give values of ρ_s for the isotropic model which are in good agreement, and which satisfy the hydrodynamic relation.

I. INTRODUCTION

The spin-wave stiffness is a parameter of fundamental importance in the spin-wave theory of quantum ferromagnets and antiferromagnets. Here we shall be particularly interested in the Heisenberg antiferromagnet. The isotropic system has a continuous rotational symmetry in spin space, which is spontaneously broken in two or three dimensions, leading to the development of Goldstone bosons, namely, the spin waves. The massless Goldstone bosons then control the behavior of the system at low energies or large distances. It has been shown[1–3] in recent years that the effects of the Goldstone bosons can be described in terms of a simple effective Lagrangian, specified purely in accordance with the symmetry properties of the model. Universal formulas can then be given for the finite-size corrections[1–5] and low-temperature corrections,[6,3] which in leading order involve just three parameters: These can be chosen as the spin-wave stiffness ρ_s, the spin-wave velocity v, and the spontaneous magnetization Σ.

There is a relationship

$$\rho_s = v^2 \chi_\perp \tag{1.1}$$

between the spin-wave stiffness, the spin-wave velocity, and the transverse susceptibility $\chi_\perp$, which was originally predicted by the "hydrodynamic" theory of Halperin and Hohenberg,[7] and a microscopic calculation of Tani.[8] The hydrodynamic theory is an early version of the effective Lagrangian theory, in fact, and the same relation indeed holds in the effective Lagrangian theory: It is expected to be exact. Equation (1.1) is often used to derive ρ_s from v and $\chi_\perp$, which are somewhat easier to calculate. It is also important, however, to calculate ρ_s directly, and verify that Eq. (1.1) is correct, as a consistency check on the whole theory. That is the purpose of the present work.

The spin-wave stiffness of the Heisenberg antiferromagnet on the square lattice has previously been calculated in spin-wave theory to order $1/(2S)^2$ (where S is the spin per site) by Igarashi and Watabe[9] and Igarashi.[10] They found that the hydrodynamic relation (1.1) was obeyed to this order. Another method of calculation was used by Singh and Huse,[11] who made a series expansion about the Ising limit. Here we extend both these approaches. In Sec. II, spin-wave perturbation theory is extended to third order for the spin-wave stiffness, using the Dyson-Maleev formalism. Results are also given for the simple cubic lattice to second order. In Sec. III, the series expansion results of Singh and Huse[11] for the square lattice are corrected and extended to tenth order in the anisotropy parameter x. The series is extrapolated to the isotropic limit $x = 1$, and the results compared with spin-wave theory. Our conclusions are summarized in Sec. IV.

II. SPIN-WAVE EXPANSION

The isotropic Heisenberg antiferromagnet can be described by the following Hamiltonian:

$$H_0 = \sum_{\langle lm \rangle} [S_l^x S_m^x + S_l^y S_m^y + S_l^z S_m^z] , \tag{2.1}$$

where $\langle lm \rangle$ denotes a sum over all nearest-neighbor pairs. The microscopic calculation of the spin-stiffness constant for this model has been discussed by Singh and Huse.[11] It involves a rotation of the order parameter by an angle θ along a given direction such as the y axis, after which we can define the stiffness constant ρ_s through the increase of the ground-state energy:

$$E_0(\theta)/N = E_0(\theta = 0)/N + \frac{1}{2}\rho_s \theta^2 + O(\theta^4) . \tag{2.2}$$

(A term linear in θ is forbidden by symmetry considerations.)

After rotation by a relative angle θ between neighboring sites along the y axis in spin space, H_0 in Eq. (2.1) becomes

$$H' = \sum_{\langle lm \rangle} [S_l^z S_m^z + S_l^x S_m^x + S_l^y S_m^y] + (\cos\theta - 1) \sum_{\langle i \rangle} (S_i^x S_{i+y}^x + S_i^z S_{i+y}^z) + \sin\theta \sum_{\langle i \rangle} S_i^z (S_{i-y}^x - S_{i+y}^x) , \tag{2.3}$$

0163-1829/94/50(10)/6877(12)/$06.00

where i runs over all lattice sites, and $i+y$ and $i-y$ indicate the nearest neighbors to the ith site in the positive and negative y directions. Expanding H' in powers of θ, and only keeping terms up to order θ^2, we get

$$\begin{aligned} H' &= \sum_{\langle lm\rangle}[S_l^z S_m^z + S_l^x S_m^x + S_l^y S_m^y] - \frac{1}{2}\theta^2 \sum_{\langle i\rangle}(S_i^x S_{i+y}^x + S_i^z S_{i+y}^z) + \theta \sum_{\langle i\rangle} S_i^z (S_{i-y}^x - S_{i+y}^x) + O(\theta^3) \\ &\equiv H_0 + H^{\text{dia}} + H^{\text{para}} + O(\theta^3) , \end{aligned} \tag{2.4}$$

where H^{dia} and H^{para} are defined by

$$H^{\text{dia}} = -\frac{1}{2}\theta^2 \sum_{\langle i\rangle}(S_i^x S_{i+y}^x + S_i^z S_{i+y}^z) , \tag{2.5}$$

$$H^{\text{para}} = \theta \sum_{\langle i\rangle} S_i^z (S_{i-y}^x - S_{i+y}^x) . \tag{2.6}$$

Thus, there are two kinds of contribution to the θ^2 part of the ground-state energy: One is the "diamagnetic" term H^{dia}, and the other is the "paramagnetic" term H^{para}.

In order to compare the results with those of the series expansion, we introduce an anisotropy parameter x to H_0 as

$$H_0 = \sum_{\langle lm\rangle}[S_l^z S_m^z + x(S_l^x S_m^x + S_l^y S_m^y)] . \tag{2.7}$$

The third-order spin-wave expansion for H_0 (obtained from a Maleev-Dyson transformation) has been discussed in our previous paper,[12] and is summarized again in the Appendix. The Hamiltonian H_0 can be expressed as

$$\begin{aligned} H = E_0 &+ \sum_k (A_k^{(1)} S + A_k^{(0)})(\alpha_k^\dagger \alpha_k + \beta_k^\dagger \beta_k) + \sum_k V_0^{(0)}(\alpha_k \beta_k + \alpha_k^\dagger \beta_k^\dagger) - \frac{z}{2N}\sum_{k_i} \delta_{\mathbf{1+2,3+4}}[V_1^{(0)}(\beta_1^\dagger \beta_2^\dagger \beta_3 \beta_4 + \alpha_3^\dagger \alpha_4^\dagger \alpha_1 \alpha_2) \\ &-2V_2^{(0)}(\alpha_3^\dagger \beta_4 \alpha_1 \alpha_2 + \alpha_4^\dagger \beta_1^\dagger \beta_2^\dagger \beta_3) - 2V_3^{(0)}(\alpha_3^\dagger \alpha_4^\dagger \alpha_2 \beta_1^\dagger + \alpha_1 \beta_2^\dagger \beta_3 \beta_4) \\ &+2V_4^{(0)}(\alpha_3^\dagger \alpha_1 \beta_2^\dagger \beta_4 + \alpha_4^\dagger \alpha_2 \beta_1^\dagger \beta_3) + V_5^{(0)}(\alpha_3^\dagger \alpha_4^\dagger \beta_1^\dagger \beta_2^\dagger + \alpha_1 \alpha_2 \beta_3 \beta_4)], \end{aligned} \tag{2.8}$$

where $\alpha_k^\dagger$, $\beta_k^\dagger$, α_k, β_k are spin-wave creation and destruction operators defined in Ref. 12, and E_0, $A_k^{(1)}$, and $A_k^{(0)}$ are

$$E_0 = -\frac{zS}{2}\left[S - C_1 + \frac{1}{4S}\left(C_1^2 + \frac{1-x^2}{x^2}(C_{-1} - C_1)^2\right)\right] , \tag{2.9a}$$

$$A_k^{(1)} = z q_k , \tag{2.9b}$$

$$A_k^{(0)} = -\frac{z}{2}[q_k C_1 + (1-x^2)\gamma_k^2 q_k^{-1}(C_{-1} - C_1)] , \tag{2.9c}$$

$$q_k = (1 - x^2\gamma_k^2)^{1/2} . \tag{2.9d}$$

Expressions for the two- and four-particle vertex factors $V_i^{(0)}$ and other quantities are given in the Appendix.

A. Diamagnetic part

The contribution to the θ^2 part of the ground-state energy from the diamagnetic term can be calculated by considering the Hamiltonian

$$H = H_0 + H^{\text{dia}} . \tag{2.10}$$

As before,[12] we first introduce boson operators via a Dyson-Maleev transformation, then perform a Fourier transformation, and finally we introduce a Bogoliubov transformation, giving

$$\begin{aligned} H^{\text{dia}} = -\frac{1}{2}\theta^2\Big\{ &- 2E_d^0 + \sum_k (\tilde{A}_k^{(1)} S + \tilde{A}_k^{(0)})(\alpha_k^\dagger \alpha_k + \beta_k^\dagger \beta_k) + \sum_k (\tilde{V}_0^{(1)} S + \tilde{V}_0^{(0)})(\alpha_k \beta_k + \alpha_k^\dagger \beta_k^\dagger) \\ &-\frac{1}{N}\sum_{k_i} \delta_{\mathbf{1+2,3+4}} \tilde{V}_5^{(0)}(\alpha_3^\dagger \alpha_4^\dagger \beta_1^\dagger \beta_2^\dagger + \alpha_1 \alpha_2 \beta_3 \beta_4) + \cdots \Big\} , \end{aligned} \tag{2.11}$$

where we have ignored the terms which do not contribute to the order considered here, and E_d^0 is the diagonal part of $H^{\rm dia}$, $\tilde{V}_0^{(1)}(k)$, $\tilde{V}_0^{(0)}(k)$ are two-particle vertices, and $\tilde{V}_5^{(0)}(\mathbf{1},\mathbf{2},\mathbf{3},\mathbf{4})$ are four-particle vertices, defined by

$$E_d^0=\frac{N}{2}\left\{S^2-\frac{S}{2x}[(2x-1)C_{-1}+C_1]+\frac{1}{4x^2}[(1-x+x^2)C_{-1}^2+(x-2)C_1C_{-1}+C_1^2]\right\}\,, \tag{2.12a}$$

$$\tilde{A}_k^{(1)}=x^{-1}\left[(2x-1)q_k^{-1}+q_k\right]\,, \tag{2.12b}$$

$$\tilde{A}_k^{(0)}=-\frac{(2-x)C_{-1}-2C_1}{2x^2}(q_k^{-1}-q_k)-\frac{(2x-1)C_{-1}+C_1}{2xq_k}\,, \tag{2.12c}$$

$$\tilde{V}_0^{(1)}(k)=[\tilde{\gamma}_k-2/(x\gamma_k)]/q_k+2q_k/(x\gamma_k)\,, \tag{2.12d}$$

$$\tilde{V}_0^{(0)}(k)=\left[\left(1-\frac{x}{2}\right)C_{-1}-C_1\right]\frac{\tilde{\gamma}_k}{xq_k}+[(2x-1)C_{-1}+C_1]\frac{q_k^{-1}-q_k}{2x^2\gamma_k}\,, \tag{2.12e}$$

$$\begin{aligned}\tilde{V}_5^{(0)}(\mathbf{1},\mathbf{2},\mathbf{3},\mathbf{4})=&\ \tilde{\gamma}_{1-4}s_1c_2s_3c_4+\tilde{\gamma}_{2-4}c_1s_2s_3c_4+\tilde{\gamma}_{1-3}s_1c_2c_3s_4+\tilde{\gamma}_{2-3}c_1s_2c_3s_4\\&-\frac{1}{2}(\tilde{\gamma}_3c_1c_2c_3s_4+\tilde{\gamma}_4c_1c_2s_3c_4+\tilde{\gamma}_3s_1s_2s_3c_4+\tilde{\gamma}_4s_1s_2c_3s_4)\,,\end{aligned} \tag{2.12f}$$

$$\begin{aligned}\tilde{\gamma}_k=&\ \frac{1}{2}\sum_{\rho=\pm y}e^{ik\cdot\rho}\\=&\left\{\begin{array}{ll}\cos\frac{a}{\sqrt{2}}(k_x+k_y), & \text{square lattice,}\\ \cos k_ya, & \text{simple cubic lattice.}\end{array}\right.\end{aligned} \tag{2.12g}$$

Here we want to calculate the contribution to the θ^2 term of the ground-state energy from the off-diagonal part of H. This can be done by using Rayleigh-Schrödinger perturbation theory: We treat the terms containing V in H as perturbation terms, and up to order S^{-1}, there are five groups of perturbation diagrams which contribute, as shown in Fig. 1. Denoting the contribution from Fig. 1(a) as E_d^a, etc., we get

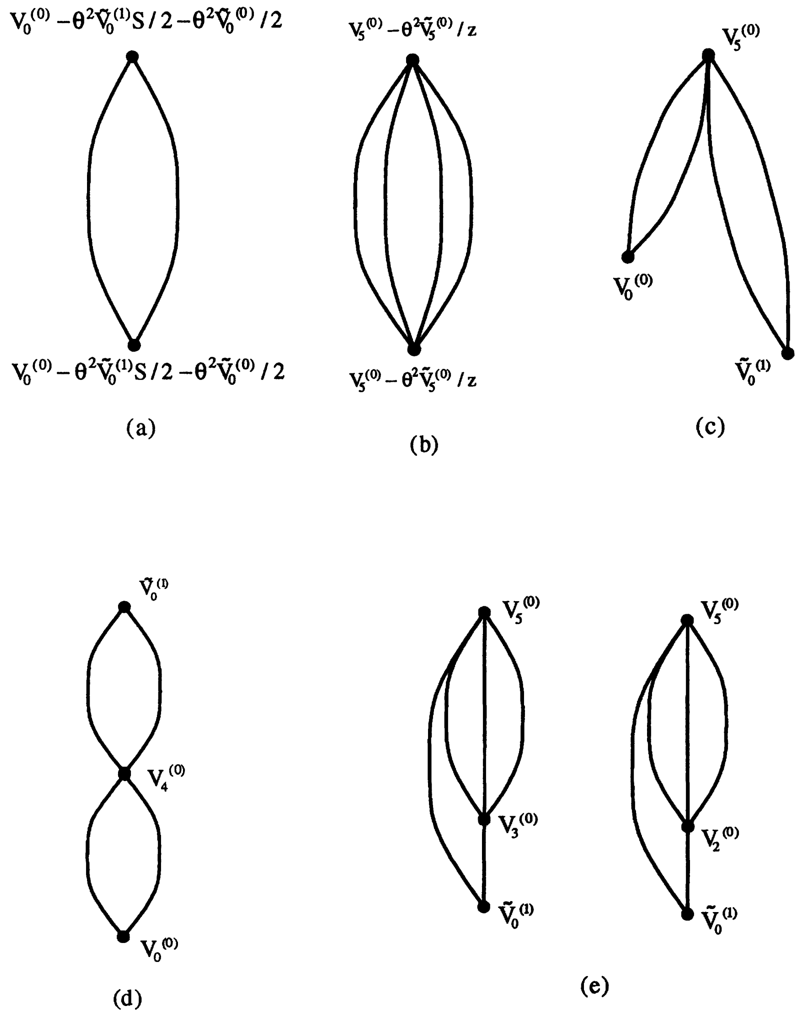

FIG. 1. The perturbation diagrams that contribute to the θ^2 part of the ground-state energy from the diamagnetic term, up to order S^{-1}. The dots represent the interaction vertices as indicated; the lines represent boson excitations in the intermediate states. To save space, we have not differentiated between the α and β bosons and possible time orderings of the vertices in the diagrams.

$$E_d^a = -\frac{1}{2}\sum_k \frac{[V_0^{(0)}(k) - \theta^2\tilde{V}_0^{(1)}(k)S/2 - \theta^2\tilde{V}_0^{(0)}(k)/2]^2}{A_k^{(1)}S + A_k^{(0)} - \theta^2\tilde{A}_k^{(1)}S/2 - \theta^2\tilde{A}_k^{(0)}/2}$$
$$\equiv E_d^a(\theta=0) + \Delta E_d^{a(0)} + \Delta E_d^{a(-1)}/S + O(S^{-2}) + O(\theta^4)\ , \tag{2.13a}$$

$$E_d^b = -\frac{zN}{8S}\left(\frac{2}{N}\right)^3 \sum_{k_i} \delta_{\mathbf{1}+\mathbf{2},\mathbf{3}+\mathbf{4}} \frac{[V_5^{(0)}(\mathbf{1},\mathbf{2},\mathbf{3},\mathbf{4}) - \frac{\theta^2}{z}\tilde{V}_5^{(0)}(\mathbf{1},\mathbf{2},\mathbf{3},\mathbf{4})][V_5^{(0)}(\mathbf{3},\mathbf{4},\mathbf{1},\mathbf{2}) - \frac{\theta^2}{z}\tilde{V}_5^{(0)}(\mathbf{3},\mathbf{4},\mathbf{1},\mathbf{2})]}{\sum_{i=1}^4 [q_i - \frac{\theta^2}{2z}\tilde{A}_i^{(0)}]}$$
$$= E_d^b(\theta=0) + \Delta E_d^b + O(\theta^4)\ , \tag{2.13b}$$

$$E_d^c = \frac{N\theta^2}{8zS}\left(\frac{2}{N}\right)^2 \sum_{k_i} \frac{V_5^{(0)}(\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{2})[V_0^{(0)}(\mathbf{1})\tilde{V}_0^{(1)}(\mathbf{2}) + V_0^{(0)}(\mathbf{2})\tilde{V}_0^{(1)}(\mathbf{1})]}{q_1(q_1+q_2)}$$
$$= \frac{N\theta^2(C_{-1}-C_1)(1-x^2)}{16xS}\left(\frac{2}{N}\right)^2 \sum_{k_i} \frac{V_5^{(0)}(\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{2})[\gamma_2\tilde{\gamma}_1 + \gamma_1\tilde{\gamma}_2 - 4x\gamma_1\gamma_2]}{q_1^2 q_2(q_1+q_2)}\ , \tag{2.13c}$$

$$E_d^d = \frac{N\theta^2}{16zS}\left(\frac{2}{N}\right)^2 \sum_{k_i} \frac{\tilde{V}_0^{(1)}(\mathbf{1})V_0^{(0)}(\mathbf{2})[V_4^{(0)}(\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{1}) + V_4^{(0)}(\mathbf{2},\mathbf{1},\mathbf{1},\mathbf{2})]}{q_1 q_2}$$
$$= \frac{N\theta^2(C_{-1}-C_1)(1-x^2)}{32xS}\left(\frac{2}{N}\right)^2 \sum_{k_i} \frac{[V_4^{(0)}(\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{1}) + V_4^{(0)}(\mathbf{2},\mathbf{1},\mathbf{1},\mathbf{2})][\gamma_2(\tilde{\gamma}_1 - 2x\gamma_1)]}{q_1^2 q_2^2}$$
$$= \frac{N}{32Sx^5}(C_{-1}-C_1)(1-x^2)(2x-1)[(C_{-3}-C_{-1})^2(x^2-1) - C_{-2}^2]\ , \tag{2.13d}$$

$$E_d^e = \frac{N\theta^2}{8S}\left(\frac{2}{N}\right)^3 \sum_{k_i} \delta_{\mathbf{1}+\mathbf{2},\mathbf{3}+\mathbf{4}} \frac{\tilde{V}_0^{(1)}(\mathbf{1})[V_2^{(0)}(\mathbf{3},\mathbf{4},\mathbf{1},\mathbf{2})V_5^{(0)}(\mathbf{1},\mathbf{2},\mathbf{3},\mathbf{4}) + V_3^{(0)}(\mathbf{2},\mathbf{1},\mathbf{3},\mathbf{4})V_5^{(0)}(\mathbf{3},\mathbf{4},\mathbf{1},\mathbf{2})]}{q_1(q_1+q_2+q_3+q_4)}\ , \tag{2.13e}$$

where $\Delta E_d^{a(0)}$, $\Delta E_d^{a(-1)}$, and ΔE_d^b are

$$\Delta E_d^{a(0)} = \frac{\theta^2}{2}\sum_k \frac{V_0^{(0)}\tilde{V}_0^{(1)}}{A_k^{(1)}}$$
$$= \frac{N\theta^2}{8x^3}(1-x^2)(C_{-1}-C_1)(C_{-1}-C_{-3})(2x-1)\ , \tag{2.14a}$$

$$\Delta E_d^{a(-1)} = \frac{\theta^2}{2}\sum_k \left[\frac{V_0^{(0)}\tilde{V}_0^{(0)}}{A_k^{(1)}} - \frac{A_k^{(0)}V_0^{(0)}\tilde{V}_0^{(1)}}{(A_k^{(1)})^2} - \frac{(V_0^{(0)})^2\tilde{A}_k^{(1)}}{2(A_k^{(1)})^2}\right]$$
$$= \frac{N\theta^2}{32x^5}(C_{-1}-C_1)^2(1-x^2)[C_{-1}(3-8x+x^2) - 2C_{-3}(3-7x-x^2+3x^3) + 3C_{-5}(1-x^2)(1-2x)]\ , \tag{2.14b}$$

$$\Delta E_d^b = -\frac{N\theta^2}{16S}\left(\frac{2}{N}\right)^3 \sum_{k_i} \delta_{\mathbf{1}+\mathbf{2},\mathbf{3}+\mathbf{4}} \left\{V_5^{(0)}(\mathbf{1},\mathbf{2},\mathbf{3},\mathbf{4})\left[V_5^{(0)}(\mathbf{3},\mathbf{4},\mathbf{1},\mathbf{2})\left(\sum_{i=1}^4 \tilde{A}_i^{(1)}\right)\right.\right.$$
$$\left.\left. -4\tilde{V}_5^{(0)}(\mathbf{3},\mathbf{4},\mathbf{1},\mathbf{2})\left(\sum_{i=1}^4 q_i\right)\right]\right\}[q_1+q_2+q_3+q_4]^{-2}\ . \tag{2.14c}$$

Up to order S^{-1}, the total θ^2 part of the ground-state energy is

$$E_d = \theta^2 E_d^0 + \Delta E_d^{a(0)} + \Delta E_d^{a(-1)} + \Delta E_d^b + E_d^c + E_d^d + E_d^e\ . \tag{2.15}$$

At the isotropic limit $x=1$, $V_0^{(0)}$ is zero, and so

$$\Delta E_d^{a(0)}/N = \Delta E_d^{a(-1)}/N = E_d^c/N = E_d^d/N = 0\ . \tag{2.16}$$

The integrations for $\Delta E_d^b/N$ and E_d^e/N are carried out in the following way: We first evaluate their values for a finite lattice, that is, sum numerically over a finite number of points distributed over the first Brillouin zone, then extrapolate the results to the infinite lattice by least-squares fitting the results to the form $E_\infty + a/L + b/L^2 + c/L^3 + \cdots$. For the square lattice, the results of integration at $x=1$ are

$$\Delta E_d^b/N = -0.059\,59(2)\theta^2/(16S)\ , \tag{2.17a}$$
$$E_d^e/N = 0.005\,532(1)\theta^2/(8S)\ . \tag{2.17b}$$

Therefore, at $x = 1$, the total contribution to the spin-stiffness constant from the diamagnetic part is

$$\rho_s^{\text{dia}} = 2E_d/(\theta^2 N)$$
$$= \begin{cases} S^2 - 0.117\,628\,254\,4S + 0.060\,415\,566\,2 - 0.006\,066(3)/S, & \text{square lattice,} \\ S^2 - 0.029\,778\,705\,69S + 0.012\,306\,389\,0, & \text{simple cubic lattice.} \end{cases} \tag{2.18}$$

B. Paramagnetic part

The contribution to the θ^2 part of the ground-state energy from the paramagnetic term can be calculated by considering the Hamiltonian

$$H = H_0 + H^{\text{para}}\ . \tag{2.19}$$

Performing the same Dyson-Maleev transformation, Fourier transformation, and Bogoliubov transformation as before, the above Hamiltonian H^{para} becomes

$$H^{\text{para}} = \theta\left(\frac{S}{N}\right)^{1/2}\sum_{k_i}\delta_{\mathbf{1+3,2}}\{\tilde{V}_1^{(\frac{1}{2})}(\alpha_2\beta_1\beta_3 + \alpha_1\alpha_3\beta_2 - \alpha_2^\dagger\beta_1^\dagger\beta_3^\dagger - \alpha_1^\dagger\alpha_3^\dagger\beta_2^\dagger)$$
$$-2\tilde{V}_2^{(\frac{1}{2})}(\alpha_2^\dagger\alpha_1\alpha_3 - \alpha_1^\dagger\alpha_3^\dagger\alpha_2 + \beta_2^\dagger\beta_1\beta_3 - \beta_1^\dagger\beta_3^\dagger\beta_2) - 2\tilde{V}_3^{(\frac{1}{2})}(\alpha_1^\dagger\alpha_2\beta_3 - \alpha_2^\dagger\alpha_1\beta_3^\dagger + \alpha_3\beta_1^\dagger\beta_2 - \beta_3^\dagger\beta_2^\dagger\beta_1)\}$$
$$+\theta\left(\frac{1}{SN}\right)^{1/2}\sum_{k_i}\delta_{\mathbf{1+3,2}}\tilde{V}^{(-\frac{1}{2})}(\alpha_1\alpha_3\beta_2 - \alpha_2^\dagger\beta_1^\dagger\beta_3^\dagger) + \cdots\ , \tag{2.20}$$

where we have again ignored the terms which do not contribute to the order considered here. As expected, there is no diagonal part for H^{para}, and the three-particle vertices $\tilde{V}_i^{(\frac{1}{2})}(\mathbf{1,2,3})$ and $\tilde{V}^{(-\frac{1}{2})}(\mathbf{1,2,3})$ are defined by

$$\tilde{V}_1^{(\frac{1}{2})}(\mathbf{1,2,3}) = \eta_3 s_1 c_2 c_3 + \eta_3 c_1 s_2 s_3 + \eta_1 c_1 c_2 s_3 + \eta_1 s_1 s_2 c_3\ , \tag{2.21a}$$
$$\tilde{V}_2^{(\frac{1}{2})}(\mathbf{1,2,3}) = (\eta_1 s_1 c_2 c_3 + \eta_1 c_1 s_2 s_3 + \eta_3 c_1 c_2 s_3 + \eta_3 s_1 s_2 c_3)/2\ , \tag{2.21b}$$
$$\tilde{V}_3^{(\frac{1}{2})}(\mathbf{1,2,3}) = \eta_3 c_1 c_2 c_3 + \eta_3 s_1 s_2 s_3 + \eta_1 c_1 s_2 c_3 + \eta_1 s_1 c_2 s_3\ , \tag{2.21c}$$
$$\tilde{V}^{(-\frac{1}{2})}(\mathbf{1,2,3}) = -\frac{C_{-1}}{2}(\eta_3 c_2 c_3 s_1 + \eta_1 c_3 s_1 s_2 + \eta_1 c_1 c_2 s_3 + \eta_3 c_1 s_2 s_3)$$
$$+\frac{C_{-1} - C_1}{2x}(-\eta_2 c_1 c_2 c_3 - \eta_2 s_1 s_2 s_3 + \eta_3 s_1 c_2 c_3 + \eta_1 s_1 s_2 c_3 + \eta_1 c_1 c_2 s_3 + \eta_3 c_1 s_2 s_3)\ , \tag{2.21d}$$
$$\eta_k = (e^{-ik\cdot\rho_y} - e^{ik\cdot\rho_y})/2$$
$$= \begin{cases} -i\sin\frac{\sqrt{2}a}{2}(k_x + k_y), & \text{square lattice,} \\ -i\sin k_y a, & \text{simple cubic lattice.} \end{cases} \tag{2.21e}$$

Again, we treat the terms containing V in the Hamiltonian $H_0 + H^{\text{para}}$ as perturbation terms, and use perturbation theory. Up to order S^{-1}, there are six groups of perturbation diagrams which contribute, as shown in Fig. 2. The contribution from each group of diagrams is

$$E_p^a = \frac{\theta^2}{z}\left(\frac{2}{N}\right)^2\sum_{k_i}\delta_{\mathbf{1+3,2}}\frac{[\tilde{V}_1^{(\frac{1}{2})}(\mathbf{1,2,3})]^2}{\sum_{i=1}^3[q_i + A_i^{(0)}/(Sz)]}$$
$$\equiv E_p^{a(0)} + E_p^{a(-1)}/S + O(S^{-2})\ , \tag{2.22a}$$
$$E_p^b = \frac{\theta^2}{zS}\left(\frac{2}{N}\right)^3\sum_{k_i}\delta_{\mathbf{1+2,5}}\delta_{\mathbf{3+4,5}}\frac{\tilde{V}_1^{(\frac{1}{2})}(\mathbf{1,5,2})\tilde{V}_2^{(\frac{1}{2})}(\mathbf{3,5,4})[V_5^{(0)}(\mathbf{1,2,3,4}) + V_5^{(0)}(\mathbf{3,4,1,2})]}{(q_1 + q_2 + q_3 + q_4)(q_1 + q_2 + q_5)}\ , \tag{2.22b}$$
$$E_p^c = \frac{2\theta^2}{zS}\left(\frac{2}{N}\right)^3\sum_{k_i}\delta_{\mathbf{1+5,3}}\delta_{\mathbf{4+5,2}}\frac{\tilde{V}_1^{(\frac{1}{2})}(\mathbf{4,2,5})\tilde{V}_3^{(\frac{1}{2})}(\mathbf{5,3,1})[V_5^{(0)}(\mathbf{1,2,3,4}) + V_5^{(0)}(\mathbf{3,4,1,2})]}{(q_1 + q_2 + q_3 + q_4)(q_2 + q_4 + q_5)}\ , \tag{2.22c}$$
$$E_p^d = \frac{\theta^2}{zS}\left(\frac{2}{N}\right)^3\sum_{k_i}\delta_{\mathbf{1+3,2}}\delta_{\mathbf{3+4,5}}\frac{\tilde{V}_1^{(\frac{1}{2})}(\mathbf{1,2,3})\tilde{V}_1^{(\frac{1}{2})}(\mathbf{3,5,4})[V_4^{(0)}(\mathbf{1,5,4,2}) + V_4^{(0)}(\mathbf{4,2,1,5})]}{(q_1 + q_2 + q_3)(q_3 + q_4 + q_5)}\ , \tag{2.22d}$$

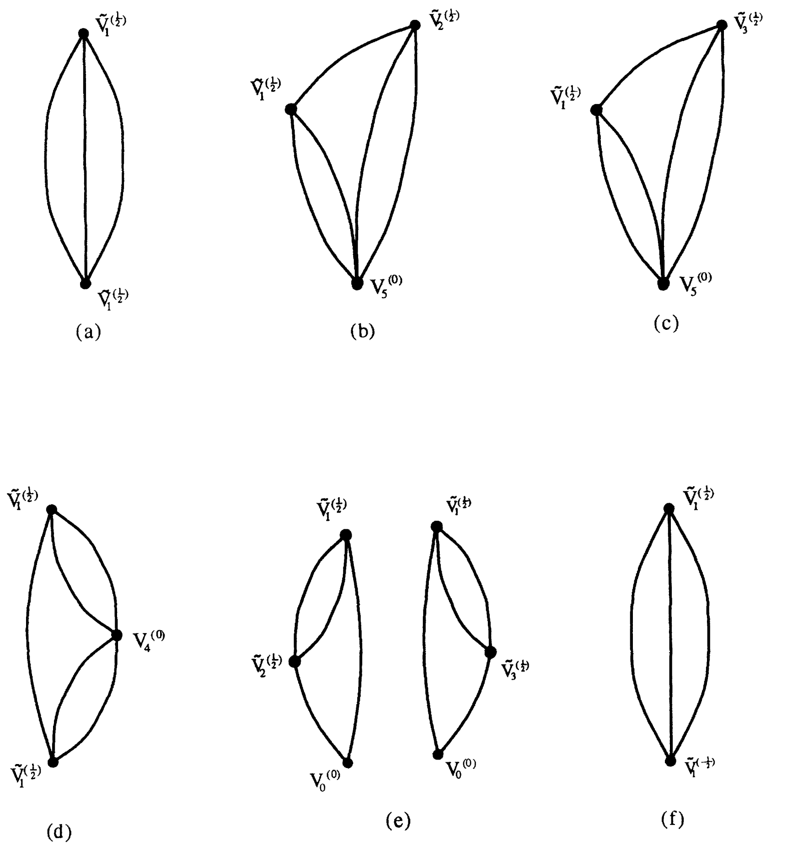

FIG. 2. The perturbation diagrams that contribute to the θ^2 part of the ground-state energy from the paramagnetic term, up to order S^{-1}.

$$E_p^e = \frac{2\theta^2}{z^2 S}\left(\frac{2}{N}\right)^2 \sum_{k_i} \delta_{\mathbf{1},\mathbf{2}+\mathbf{3}} \frac{\tilde{V}_1^{(\frac{1}{2})}(\mathbf{2},\mathbf{1},\mathbf{3})}{q_1+q_2+q_3}\left\{\frac{\tilde{V}_2^{(\frac{1}{2})}(\mathbf{2},\mathbf{1},\mathbf{3})V_0^{(0)}(\mathbf{1})}{q_1} + \frac{\tilde{V}_3^{(\frac{1}{2})}(\mathbf{2},\mathbf{1},\mathbf{3})V_0^{(0)}(\mathbf{2})}{q_2}\right\}$$

$$= \frac{2(C_{-1}-C_1)(1-x^2)\theta^2}{2xzS}\left(\frac{2}{N}\right)^2 \sum_{k_i} \delta_{\mathbf{1},\mathbf{2}+\mathbf{3}} \frac{\tilde{V}_1^{(\frac{1}{2})}(\mathbf{2},\mathbf{1},\mathbf{3})}{q_1+q_2+q_3}\left\{\frac{\gamma_1\tilde{V}_2^{(\frac{1}{2})}(\mathbf{2},\mathbf{1},\mathbf{3})}{q_1^2} + \frac{\gamma_2\tilde{V}_3^{(\frac{1}{2})}(\mathbf{2},\mathbf{1},\mathbf{3})}{q_2^2}\right\}, \quad (2.22e)$$

$$E_p^f = \frac{\theta^2}{zS}\left(\frac{2}{N}\right)^2 \sum_{k_i} \delta_{\mathbf{2},\mathbf{1}+\mathbf{3}} \frac{\tilde{V}_1^{(\frac{1}{2})}(\mathbf{1},\mathbf{2},\mathbf{3})\tilde{V}^{(-\frac{1}{2})}(\mathbf{1},\mathbf{2},\mathbf{3})}{q_1+q_2+q_3}, \quad (2.22f)$$

where $E_p^{a(0)}$ and $E_p^{a(-1)}$ are defined as

$$E_p^{a(0)} = \frac{\theta^2}{z}\left(\frac{2}{N}\right)^2 \sum_{k_i} \delta_{\mathbf{1}+\mathbf{3},\mathbf{2}} \frac{[\tilde{V}_1^{(\frac{1}{2})}(\mathbf{1},\mathbf{2},\mathbf{3})]^2}{q_1+q_2+q_3}, \quad (2.23a)$$

$$E_p^{a(-1)} = -\frac{\theta^2}{z^2}\left(\frac{2}{N}\right)^2 \sum_{k_i} \delta_{\mathbf{1}+\mathbf{3},\mathbf{2}} \frac{[\tilde{V}_1^{(\frac{1}{2})}(\mathbf{1},\mathbf{2},\mathbf{3})]^2 \sum_{i=1}^3 A_i^{(0)}}{(q_1+q_2+q_3)^2}. \quad (2.23b)$$

Up to order S^{-1}, the total θ^2 part of the ground-state energy is

$$E_p = E_p^a + E_p^b + E_p^c + E_p^d + E_p^e + E_p^f. \quad (2.24)$$

At the isotropic limit $x = 1$,

$$E_p^e/N = 0. \quad (2.25)$$

The integrations for other quantities are carried out in the same way as before, and for the square lattice, the results are (at $x = 1$):

$$E_p^a/N = (-0.141\,247\,107/z)\left(1+\frac{C_1}{2S}\right)\theta^2 , \tag{2.26a}$$

$$E_p^b/N = 0.003\,875(1)\theta^2/(zS) , \tag{2.26b}$$

$$E_p^c/N = -0.009\,38(1)(2\theta^2)/(zS) , \tag{2.26c}$$

$$E_p^d/N = -0.029\,87(2)\theta^2/(zS) , \tag{2.26d}$$

$$E_p^f/N = 0.039\,403\,6(10)\theta^2/(zS) . \tag{2.26e}$$

For the simple cubic lattice, the result for $E_p^{a(0)}$ is

$$E_p^{a(0)}/N = -0.039\,444\,9(2)\theta^2/z . \tag{2.27}$$

Therefore, the total contribution to the spin-stiffness constant from the paramagnetic part is

$$\rho_s^{\text{para}} = 2E_p/(\theta^2 N)$$

$$= \begin{cases} -0.070\,623\,553\,5 + 0.002\,90(2)/S, & \text{square lattice,} \\ -0.013\,148\,3(1), & \text{simple cubic lattice.} \end{cases} \tag{2.28}$$

Therefore, the spin-stiffness constant is

$$\rho_s = \rho_s^{\text{dia}} + \rho_s^{\text{para}}$$

$$= \begin{cases} S^2 - 0.117\,628\,254\,4S - 0.010\,207\,987\,3 - 0.003\,16(2)/S, & \text{square lattice,} \\ S^2 - 0.029\,778\,705\,69S - 0.000\,841\,9(1), & \text{simple cubic lattice.} \end{cases} \tag{2.29}$$

These results will be compared with the hydrodynamic relation (1.1) in Sec. IV.

III. SERIES EXPANSION

In an earlier paper[13] we derived series expansions for the ground-state energy and other properties of the Heisenberg antiferromagnet on the square lattice. The basic approach uses a method due to Nickel,[14] which has been described in some detail by He *et al.*[15] The starting point is a list of all connected clusters $\{\alpha\}$ up to some order, and their embedding constants C_α^N for the lattice of interest. The ground-state energy is then expressed as

$$E_0^N = \sum_\alpha C_\alpha^N \varepsilon_\alpha, \tag{3.1}$$

where the quantities ε_α are obtained recursively.

The major difference between the present calculation and our previous work is that the (x,y) symmetry of the lattice is broken by the imposed twist in the Hamiltonian. This greatly increases the number of clusters which must be considered, since realizations which are related by 90° rotations or diagonal reflections are no longer equivalent and must be distinguished. For the square lattice, for example, there are 1248 distinct topologies with up to 11 sites but 46 924 inequivalent space types.

As discussed in the previous section, the spin-wave stiffness ρ_s can be computed through the following Hamiltonian:

$$\begin{aligned} H = & \sum_{\langle lm\rangle}[S_l^z S_m^z + x(S_l^x S_m^x + S_l^y S_m^y)] \\ & -\frac{h_1}{2}\sum_{\langle i\rangle}(S_i^x S_{i+y}^x + S_i^z S_{i+y}^z) \\ & +h_2\sum_{\langle i\rangle} S_i^z(S_{i-y}^x - S_{i+y}^x). \end{aligned} \tag{3.2}$$

The spin-wave stiffness is then obtained, as a series in x, from $\rho_s = \rho_s^{\text{dia}} + \rho_s^{\text{para}}$, with

$$\rho_s^{\text{dia}} = \frac{2}{N}\frac{\partial E_0}{\partial h_1}\bigg|_{h_1=h_2=0} , \tag{3.3}$$

$$\rho_s^{\text{para}} = \frac{1}{N}\frac{\partial^2 E_0}{\partial h_2^2}\bigg|_{h_1=h_2=0} . \tag{3.4}$$

By a spin rotation on the odd sublattice m, the Hamiltonian can be transformed to

$$\begin{aligned} H = & -\sum_{\langle lm\rangle}[S_l^z S_m^z - \frac{x}{2}(S_l^+ S_m^+ + S_l^- S_m^-)] \\ & +\frac{h_1}{2}\sum_{\langle i\rangle}(S_i^z S_{i+y}^z - S_i^x S_{i+y}^x) \\ & +h_2\Big[\sum_{\langle m\rangle} S_m^x(S_{m+y}^z \\ & -S_{m-y}^z) - \sum_{\langle l\rangle} S_l^x(S_{l+y}^z - S_{l-y}^z)\Big]. \end{aligned} \tag{3.5}$$

The unperturbed ground state has all spins "up" and the

TABLE I. Coefficients of series expansions in x for the spin-stiffness constant ρ_s of the spin-$\frac{1}{2}$ and spin-1 Heisenberg antiferromagnets on a square lattice.

Order	$S=\frac{1}{2}$	$S=1$
0	1/4	1
1	$8.333333333333\times10^{-2}$	$1.428571428571\times10^{-1}$
2	$-9.722222222222\times10^{-2}$	$-1.551020408163\times10^{-1}$
3	$-1.481481481481\times10^{-2}$	$2.114823951559\times10^{-2}$
4	$-3.285751028807\times10^{-3}$	$-4.316225020525\times10^{-2}$
5	$1.273797276112\times10^{-3}$	$7.497565665159\times10^{-3}$
6	$-5.636489572877\times10^{-3}$	$-2.107081657979\times10^{-2}$
7	$-2.379164748374\times10^{-4}$	$4.488596116436\times10^{-3}$
8	$-4.262931924240\times10^{-3}$	$-1.353720806360\times10^{-2}$
9	$-3.113622337613\times10^{-4}$	$3.002732498636\times10^{-3}$
10	$-2.317964076705\times10^{-3}$	$-9.571728250082\times10^{-3}$

operator proportional to x is treated as a perturbation which flips both spins on a bond $\langle lm\rangle$.

We have carried out the calculation for the square lattice only, which involves a total of 46 924 linked clusters, as mentioned above. The resulting series for both spin-$\frac{1}{2}$ and spin-1 models are listed in Table I. The only previous expansion of which we are aware is that of Singh and Huse[11] for $S=\frac{1}{2}$. Our series coefficients differ from theirs already at order x, although the difference between the two series appears to be proportional to $(1-x)$, so that they give similar results at the isotropic point $x=1$. As a check on our results, one can perform a series expansion of the spin-wave predictions at first and second order, for $S=\frac{1}{2}$:

$$\rho_s^{1\text{st}}=0.25+0.0625x-0.0625x^2+0.017\,578\,125x^3-0.026\,367\,187\,5x^4+0.009\,155\,2x^5+\cdots\,, \tag{3.6a}$$

$$\rho_s^{2\text{nd}}=0.25+0.078\,125x-0.088\,541\,67x^2+0.011\,718\,75x^3-0.024\,726x^4+0.003\,148\,4x^5+\cdots\,. \tag{3.6b}$$

These appear to be converging towards the series given in Table I, for at least the first three terms. We also obtain three more terms than Singh and Huse[11] for the $S=\frac{1}{2}$ case, and present new series for $S=1$.

Now a series in x has already been calculated for the transverse susceptibility $\chi_\perp$ in a previous paper.[13] No such series exists for the spin-wave velocity v, and the hydrodynamic relation (1.1) only holds when $x=1$. Nevertheless, we can get a better estimate of v by generating a new series for the quantity $\Lambda(x)$ defined as

$$\Lambda(x)=\rho_s(x)\chi_\perp^{-1}(x)\,, \tag{3.7}$$

such that as $x\to1$, $\Lambda(x)\to v^2$. The series coefficients for $\Lambda(x)$ are listed in Table II.

According to spin-wave theory, the asymptotic expansion near $x=1$ for both the spin-wave stiffness ρ_s and transverse susceptibility $\chi_\perp$ should have the form

$$\rho_s(x)=\rho_0+\rho_1(1-x)^{1/2}+\rho_2(1-x)+\cdots, \tag{3.8a}$$

$$\chi_\perp(x)=\chi_0+\chi_1(1-x)^{1/2}+\chi_2(1-x)+\cdots, \tag{3.8b}$$

while $\Lambda(x)$ should behave as

$$\Lambda(x)=\Lambda_0+\Lambda_1(1-x)+\Lambda_2(1-x)^{3/2}+\Lambda_3(1-x)^2+\cdots. \tag{3.9}$$

TABLE II. Coefficients of series expansions in x for $\Lambda(x)=\rho_s(x)/\chi_\perp(x)$ of the spin-$\frac{1}{2}$ and spin-1 Heisenberg antiferromagnets on a square lattice.

Order	$S=\frac{1}{2}$	$S=1$
0	1	4
1	5/3	36/7
2	$4.166666666667\times10^{-1}$	$6.285714285714\times10^{-1}$
3	$-3.462962962963\times10^{-1}$	$-3.507512895268\times10^{-1}$
4	$-6.837397119342\times10^{-2}$	$4.560329228719\times10^{-2}$
5	$5.305307172252\times10^{-2}$	$-5.820911372281\times10^{-2}$
6	$1.758096625782\times10^{-2}$	$6.868291686964\times10^{-3}$
7	$2.714959220121\times10^{-3}$	$-1.450772495242\times10^{-2}$
8	$7.836572054946\times10^{-3}$	$4.578594070967\times10^{-3}$
9	$-2.164866993509\times10^{-3}$	$-7.482126592187\times10^{-3}$
10	$-4.109975940784\times10^{-3}$	$2.626020853309\times10^{-3}$

Note that in order for the $(1-x)^{1/2}$ term in (3.9) to vanish, the ratios χ_1/χ_0 and ρ_1/ρ_0 must be equal, by Eq. (3.7). This also follows from the hypothesis of universal amplitude ratios discussed by Singh and Huse.[11]

The analysis of these series proceeded as follows. After promoting the singular term in $(1-x)$ to leading order by differentiating the series, a standard Dlog Padé analysis showed that the singular point indeed lies near $x = 1$, with a critical index which is by and large consistent with the spin-wave predictions, although the estimate is not very accurate.

To estimate the leading order coefficient in the asymptotic expansion (such as ρ_0 or Λ_0), we first[16] transform to a new variable $\delta = 1-(1-x)^{1/2}$, so that according to spin-wave theory, the function should be analytic in δ. Next, the series is extrapolated to the point $\delta = 1$ (or $x = 1$) by using an integrated first-order inhomogeneous differential approximant.[17]

To estimate the next-to-leading coefficient (such as ρ_1, Λ_1, and Λ_2), we have trivially derived series for the following quantities, with the expected asymptotic behavior as listed:

$$-2(1-x)^{1/2}\frac{d\rho_s}{dx} = \rho_1 + 2\rho_2(1-x)^{1/2} + 3\rho_3(1-x) + \cdots, \tag{3.10a}$$

$$-\frac{d\Lambda}{dx} = \Lambda_1 + 3\Lambda_2(1-x)^{1/2}/2 + 2\Lambda_3(1-x) + \cdots, \tag{3.10b}$$

$$\frac{4}{3}(1-x)^{1/2}\frac{d^2\Lambda}{dx^2} = \Lambda_2 + 8\Lambda_3(1-x)^{1/2}/3 + \cdots. \tag{3.10c}$$

The method of analysis is the same as above.

The resulting estimates for the spin-wave stiffness ρ_s are

$$\begin{aligned}\rho_s &= \begin{cases} 0.182(5) + 0.14(2)(1-x)^{1/2} + \cdots, & S = \frac{1}{2}, \\ 0.872(4) + 0.364(10)(1-x)^{1/2} + \cdots, & S = 1, \end{cases} \\ &= \begin{cases} 0.182(5)[1 + 0.54(7)(1-x^2)^{1/2} + \cdots], & S = \frac{1}{2}, \\ 0.872(4)[1 + 0.297(8)(1-x^2)^{1/2} + \cdots], & S = 1, \end{cases}\end{aligned} \tag{3.11}$$

and for $\Lambda(x)$

$$\Lambda(x) = \begin{cases} 2.74(4) - 1.99(10)(1-x) + 1.2(4)(1-x)^{3/2} + \cdots, & S = \frac{1}{2}, \\ 9.398(4) - 4.8(2)(1-x) - 1.2(3)(1-x)^{3/2} + \cdots, & S = 1. \end{cases} \tag{3.12}$$

Therefore the spin-wave velocity v for the isotropic Heisenberg antiferromagnet is

$$v = \sqrt{\Lambda(1)} = \begin{cases} 1.655(12), & S = \frac{1}{2}, \\ 3.0656(7), & S = 1. \end{cases} \tag{3.13}$$

Estimates for the transverse susceptibility were obtained previously,[13]

$$\begin{aligned}\chi_\perp &= \begin{cases} 0.0659(10) + 0.037(3)(1-x^2)^{1/2} + \cdots, & S = \frac{1}{2}, \\ 0.0925(10) + 0.031(6)(1-x^2)^{1/2} + \cdots, & S = 1, \end{cases} \\ &= \begin{cases} 0.0659(10)[1 + 0.56(6)(1-x^2)^{1/2} + \cdots], & S = \frac{1}{2}, \\ 0.0925(10)[1 + 0.34(6)(1-x^2)^{1/2} + \cdots], & S = 1. \end{cases}\end{aligned} \tag{3.14}$$

These should be compared with the predictions of the spin-wave theory of Sec. II:

$$\text{first order}: \quad \rho_s = \begin{cases} 0.191\,186, & S = \frac{1}{2} \\ 0.882\,372, & S = 1; \end{cases} \tag{3.15}$$

$$\text{second order}: \quad \rho_s = \begin{cases} 0.180\,978, & S = \frac{1}{2}, \\ 0.872\,164, & S = 1; \end{cases} \tag{3.16}$$

$$\text{third order}: \quad \rho_s = \begin{cases} 0.174\,66(4), & S = \frac{1}{2}, \\ 0.869\,00(2), & S = 1. \end{cases} \tag{3.17}$$

The agreement between (3.17) and (3.11) is quite reasonable, and the ratios χ_1/χ_0 and ρ_1/ρ_0 are equal within the range of error.

A comparison of estimates obtained for ρ_s from spin-wave theory and from series extrapolations is shown in Fig. 3, graphed against the anisotropy parameter δ. It can be seen that the third-order spin-wave prediction agrees very well with the series extrapolation, except perhaps at the isotropic point $\delta = 1$. The accuracy of both estimates appears quite similar at the isotropic point.

IV. SUMMARY AND CONCLUSIONS

The spin-wave stiffness of the isotropic Heisenberg antiferromagnet has been calculated in spin-wave perturbation theory as

$$\rho_s = S^2 - 0.117\,628\,254\,4S - 0.010\,207\,987\,3 - 0.003\,16(2)/S + O(S^{-2}), \text{ square lattice,} \quad (4.1a)$$

$$\rho_s = S^2 - 0.029\,778\,705\,69S - 0.000\,841\,9(1) + O(S^{-1}), \quad \text{simple cubic lattice.} \quad (4.1b)$$

The first three terms of (4.1a) were determined previously by Igarashi and Watabe[9] and Igarashi.[10] Corresponding results for the spin-wave velocity are

$$v = 2\sqrt{2}S\left[1 + \frac{0.157\,947\,421}{2S} + \frac{0.021\,52(2)}{(2S)^2} + O(S^{-3})\right], \quad \text{square lattice,} \quad (4.2a)$$

$$v = 2\sqrt{3}S\left[1 + \frac{0.097\,158\,004}{2S} + \frac{0.005\,06(8)}{(2S)^2} + O(S^{-3})\right], \quad \text{simple cubic lattice.} \quad (4.2b)$$

The result (4.2a) was obtained by Igarashi,[10] Canali, Girvin, and Wallin,[18] and Zheng and Hamer.[19] For the transverse susceptibility, we have

$$\chi_\perp = 1/8 - 0.034\,446\,959\,42/S + 0.002\,040\,06(7)/S^2 + O(S^{-3}), \quad \text{square lattice,} \quad (4.3a)$$

$$\chi_\perp = 1/12 - 0.010\,578\,058\,5/S + 0.000\,550\,005(20)/S^2 + O(S^{-3}), \quad \text{simple cubic lattice,} \quad (4.3b)$$

where (4.3a) was first obtained by Igarashi.[10] A slightly different result was obtained by Hamer, Zheng, and Arndt,[12] due to the erroneous use of a perturbed energy rather than an unperturbed energy in a denominator of their Eq. (2.57). If the term $m^{(-1)}$ is removed from this equation, the result is that given above, and agrees with that of Igarashi.[10]

It is now easy to verify that the hydrodynamic relation (1.1) is precisely satisfied by Eqs. (4.1)–(4.3) through second order in S^{-1}, for both the square and simple cubic lattices. This provides strong evidence that the spin-wave calculations are correct and consistent.

For the square lattice case, we have also calculated a series expansion about the Ising limit, following Singh and Huse,[11] and extrapolated to the isotropic limit to obtain

$$\rho_s = \begin{cases} 0.182(5) + 0.14(2)(1-x)^{1/2} + \cdots, & S = \frac{1}{2}, \\ 0.872(4) + 0.364(10)(1-x)^{1/2} + \cdots, & S = 1, \end{cases} \quad (4.4)$$

which agrees to within 4% with the spin-wave prediction (4.1). A similar method applied to the transverse susceptibility[13] gave

$$\chi_\perp = \begin{cases} 0.0659(10) + 0.037(3)(1-x^2)^{1/2} + \cdots, & S = \frac{1}{2}, \\ 0.0925(10) + 0.031(6)(1-x^2)^{1/2} + \cdots, & S = 1, \end{cases} \quad (4.5)$$

which agrees with (4.3) to within 2%. Combining the series for ρ_s and $\chi_\perp$ gives

$$v = \begin{cases} 1.655(12), & S = \frac{1}{2}, \\ 3.0656(7), & S = 1, \end{cases} \quad (4.6)$$

which agrees with (4.2) to 1%.

A Monte Carlo estimate of the spin-wave stiffness has been made by Makivic and Ding.[20] They obtained $\rho_s =$ 0.199(2) for the $S = \frac{1}{2}$ model on a square lattice, to be compared with our results $\rho_s = 0.175(6)$ (spin wave) and $\rho_s = 0.182(5)$ (series). Igarashi[10] had already obtained $\rho_s \simeq 0.181$ from the second-order spin-wave expansion. It can be seen that the estimate of Makivic and Ding[20] lies somewhat higher than the series or spin-wave results.

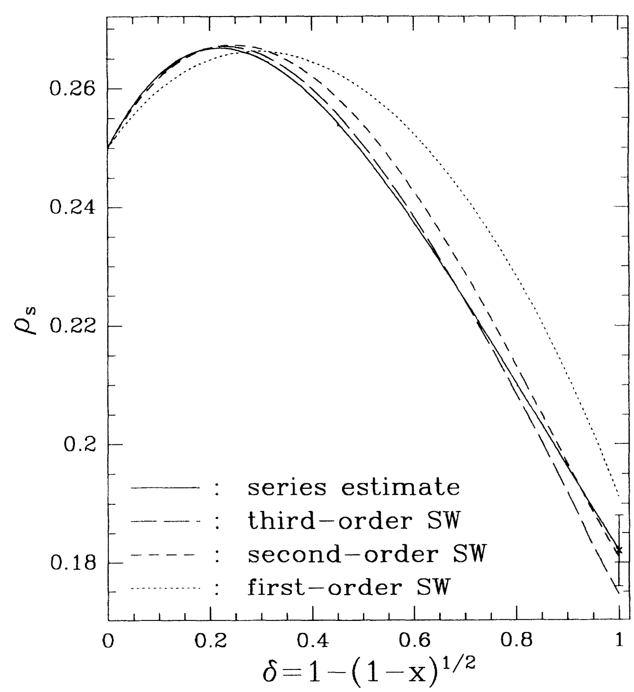

FIG. 3. Graph of the spin-stiffness constant ρ_s against $\delta = 1 - (1-x)^{1/2}$ for the spin-$\frac{1}{2}$ Heisenberg antiferromagnet on the square lattice. The four curves shown are the series estimate, and the first-, second-, and third-order spin-wave predictions corresponding to solid, dotted, short dashed, and long dashed lines, respectively. The error at $x = 1$ from the series estimate is also marked.

ACKNOWLEDGMENT

This work forms part of a research project supported by a grant from the Australian Research Council.

APPENDIX

The spin-wave expansion for H_0 is accomplished by the three following transformations. First we introduce boson operators a_l and b_m via the Dyson-Maleev transformation on the two sublattices:

$$\begin{aligned} &l \text{ sublattice}: \; S_l^z = S - a_l^\dagger a_l,\; S_l^+ = (2S)^{1/2} a_l - (2S)^{-1/2} a_l^\dagger a_l a_l,\; S_l^- = (2S)^{1/2} a_l^\dagger; \\ &m \text{ sublattice}: \; S_m^z = b_m^\dagger b_m - S,\; S_m^+ = (2S)^{1/2} b_m^\dagger - (2S)^{-1/2} b_m^\dagger b_m^\dagger b_m,\; S_m^- = (2S)^{1/2} b_m . \end{aligned} \tag{A1}$$

In terms of the boson operators, the Hamiltonian can be expressed as

$$\begin{aligned} H_0 = -NS^2 z/2 + zS \sum_l a_l^\dagger a_l + zS \sum_m b_m^\dagger b_m + xS \sum_{\langle lm\rangle} (a_l b_m + a_l^\dagger b_m^\dagger) \\ - \sum_{\langle lm\rangle} a_l^\dagger a_l b_m^\dagger b_m - \frac{x}{2} \sum_{\langle lm\rangle} (a_l^\dagger a_l a_l b_m + a_l^\dagger b_m^\dagger b_m^\dagger b_m) \, . \end{aligned} \tag{A2}$$

Then, we can introduce the Bloch-type boson operators a_k, b_k by a Fourier transformation:

$$a_k = \left(\frac{2}{N}\right)^{1/2} \sum_l e^{ik\cdot l} a_l, \quad b_k = \left(\frac{2}{N}\right)^{1/2} \sum_m e^{-ik\cdot m} b_m, \tag{A3}$$

where N is the total number of lattice sites. The quadratic part of H_0 can be diagonalized by a Bogoliubov transformation:

$$\begin{aligned} a_k &= \alpha_k \cosh\theta_k - \beta_k^\dagger \sinh\theta_k, \\ b_k &= -\alpha_k^\dagger \sinh\theta_k + \beta_k \cosh\theta_k, \end{aligned} \tag{A4}$$

where $\tanh 2\theta_k = x\gamma_k$, z is the coordination number of the lattice (i.e., 4 for the square lattice), and γ_k is the structure factor:

$$\gamma_k = \frac{1}{z} \sum_\rho e^{ik\cdot\rho} \, . \tag{A5}$$

After this transformation, the Hamiltonian now has the form given in Eq. (2.8), with the following two- and four-particle Dyson-Maleev vertex factors $V_i^{(0)}(\mathbf{1},\mathbf{2},\mathbf{3},\mathbf{4})$ $(i = 0, \ldots, 5)$:

$$\begin{aligned} V_0^{(0)} &= \frac{z}{2x}(1-x^2)(C_{-1} - C_1)\gamma_k(1 - x^2\gamma_k^2)^{-1/2}, \\ V_1^{(0)} &= \gamma_{3-2} c_1 s_2 s_3 c_4 + \gamma_{3-1} s_1 c_2 s_3 c_4 + \gamma_{4-2} c_1 s_2 c_3 s_4 + \gamma_{4-1} s_1 c_2 c_3 s_4 \\ &\quad - x(\gamma_3 s_1 s_2 c_3 s_4 + \gamma_4 s_1 s_2 s_3 c_4 + \gamma_4 c_1 c_2 c_3 s_4 + \gamma_3 c_1 c_2 s_3 c_4), \\ V_2^{(0)} &= \gamma_{4-2} c_1 s_2 c_3 c_4 + \gamma_{4-1} s_1 c_2 c_3 c_4 + \gamma_{3-2} c_1 s_2 s_3 s_4 + \gamma_{3-1} s_1 c_2 s_3 s_4 \\ &\quad - x(\gamma_3 s_1 s_2 c_3 c_4 + \gamma_4 s_1 s_2 s_3 s_4 + \gamma_4 c_1 c_2 c_3 c_4 + \gamma_3 c_1 c_2 s_3 s_4), \\ V_3^{(0)} &= \gamma_{4-1} c_1 c_2 c_3 s_4 + \gamma_{3-1} c_1 c_2 s_3 c_4 + \gamma_{3-2} s_1 s_2 s_3 c_4 + \gamma_{4-2} s_1 s_2 c_3 s_4 \\ &\quad - x(\gamma_3 c_1 s_2 c_3 s_4 + \gamma_4 c_1 s_2 s_3 c_4 + \gamma_4 s_1 c_2 c_3 s_4 + \gamma_3 s_1 c_2 s_3 c_4), \\ V_4^{(0)} &= \gamma_{4-2} c_1 c_2 c_3 c_4 + \gamma_{3-2} c_1 c_2 s_3 s_4 + \gamma_{4-1} s_1 s_2 c_3 c_4 + \gamma_{3-1} s_1 s_2 s_3 s_4 \\ &\quad - x(\gamma_3 s_1 c_2 c_3 c_4 + \gamma_4 s_1 c_2 s_3 s_4 + \gamma_4 c_1 s_2 c_3 c_4 + \gamma_3 c_1 s_2 s_3 s_4), \\ V_5^{(0)} &= \gamma_{4-2} s_1 c_2 c_3 s_4 + \gamma_{4-1} c_1 s_2 c_3 s_4 + \gamma_{4-1} s_1 c_2 s_3 c_4 + \gamma_{3-1} c_1 s_2 s_3 c_4 \\ &\quad - x(\gamma_3 s_1 s_2 s_3 c_4 + \gamma_4 s_1 s_2 c_3 s_4 + \gamma_4 c_1 c_2 s_3 c_4 + \gamma_3 c_1 c_2 s_3 c_4), \end{aligned} \tag{A6}$$

where s_i and c_i denote $\sinh\theta_{k_i}$ and $\cosh\theta_{k_i}$, respectively, and C_n is defined by

$$C_n = \frac{2}{N} \sum_k \left[(1 - x^2\gamma_k^2)^{n/2} - 1\right]. \tag{A7}$$

* Electronic address: c.hamer@unsw.edu.au
† Electronic address: w.zheng@unsw.edu.au
‡ Electronic address: otja@newt.phys.unsw.edu.au

[1] H. Neuberger and T. Ziman, Phys. Rev. B **39**, 2608 (1989).
[2] D.S. Fisher, Phys. Rev. B **39**, 11783 (1989).
[3] P. Hasenfratz and F. Niedermayer (unpublished).
[4] M.E. Fisher and V. Privman, Phys. Rev. B **32**, 447 (1985).
[5] P. Hasenfratz and H. Leutwyler, Nucl. Phys. **B343**, 241 (1990).
[6] J.M. Luck, J. Phys. A **15**, L169 (1982).
[7] B.I. Halperin and P.C. Hohenberg, Phys. Rev. **188**, 898 (1969).
[8] K. Tani, Prog. Theor. Phys. **31**, 335 (1964).
[9] J. Igarashi and A. Watabe, Phys. Rev. B **44**, 5057 (1991).
[10] J. Igarashi, Phys. Rev. B **46**, 10763 (1992).
[11] R.R.P. Singh and D.A. Huse, Phys. Rev. B **40**, 7247 (1989).
[12] C.J. Hamer, W.H. Zheng, and Peter Arndt, Phys. Rev. B **46**, 6276 (1992).
[13] W.H. Zheng, J. Oitmaa, and C.J. Hamer, Phys. Rev. B **43**, 8321 (1991).
[14] B.G. Nickel (unpublished).
[15] H.X. He, C.J. Hamer, and J. Oitmaa, J. Phys. A **23**, 1775 (1990).
[16] D.A. Huse, Phys. Rev. B **37**, 2380 (1988).
[17] A.J. Guttmann, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. Lebowitz (Academic, New York, 1989), Vol. 13.
[18] C.M. Canali, S.M. Girvin, and M. Wallin, Phys. Rev. B **45**, 10131 (1992).
[19] W.H. Zheng and C.J. Hamer, Phys. Rev. B **47**, 7961 (1993).
[20] M.S. Makivic and H.Q. Ding, Phys. Rev. B **43**, 3562 (1991).