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# Schwinger-boson mean-field theory of spin-$\frac{1}{2}$ 2D antiferromagnet

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**Abstract.** A consistent Schwinger-boson mean field theory is developed for a spin-$\frac{1}{2}$ 2D antiferromagnet. It predicts that there are two branches of the Schwinger-boson excitation spectrum: an acoustic branch, essentially the same as that predicted by Arovas and Auerbach theory, and a new optical branch. The present theory provides a natural explanation of the mystery of the Raman "two magon" scattering from $La_2CuO_4$.

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In the past six years, intensive investigation on the magnetic properties of $La_2CuO_4$ (and other parent compounds of the High $T_c$ cuprates) have been made with the aim to understand the mystery of the high $T_c$ cuprate [1, 2]. Thermal neutron scattering on $La_2CuO_4$ [3] shows that it is a quasi two-dimensional $(2D)$ spin-$\frac{1}{2}$ antiferromagntism with spin wave as its low energy excitation, consistent with the conventional spin wave theory (cSWT) [4]. The peculiarity of spin-$\frac{1}{2}$ antiferromagneuism lies in that there are also experiments such as the "two-magnon" Raman scattering from $La_2CuO_4$ [5–7] which cannot be explained by the theory based on the cSWT, in spite of such theory is fitted very well with that from $S \geq 1$ antiferromagnetic materials [8, 9]. This failure probably hints that the cSWT does not represent the whole story for spin-$\frac{1}{2}$ $2D$ antiferromagnet. In the present letter, we reexamine the Schwinger-boson mean-field theory of antiferromagnetism and show that there is a new branch of boson excitation missed in the cSWT.

Arovas and Auerbach (AA) [10] first developed a Schwinger boson theory of the $SU(N)$ generalization of the Heisenberg model. They formulated their theory in the functional form. And in the saddle point approximation they have studied the thermodynamic and dynamic properties of the low dimensional ferromagnet and antiferromagnet in the low temperature and disordered regime. Sarker et al. [11] showed later that the results of AA can be obtained easily by a mean field decomposition of the Heisenberg Hamiltonian into a quadratic form. They argued that the magnetic ordering is identified with the Bose condensation of the Schwinger bosons, and extended AA theory to cover the magnetic long range order regime. In their mean field decomposition they only consider the anomalous contractions of the Schwinger bosons $\langle b^+ b^+ \rangle$ and $\langle bb \rangle$. Yoshioka showed in the paper [12] that the inclusion of the normal contractions leads only to an unimportant renormalization of the parameters in the theory. However, it is in general not true. In a consistent mean field theory, the normal contractions also play an important role.

Consider a spin-$\frac{1}{2}$ Heisenberg antiferromagnet on a square lattice. Following the work of Sarker et al. [11], we start our study from the Hamiltonian

$$H = \tfrac{1}{2} NJ - \tfrac{1}{2} J \sum_{\langle ij \rangle} \sum_{\sigma} b^{\dagger}_{j\sigma} b^{\dagger}_{i\sigma} b_{i\sigma} b_{j\sigma} - \tfrac{1}{2} J \sum_{\langle ij \rangle} \sum_{\sigma} b^{\dagger}_{j\sigma} b^{\dagger}_{i\sigma} b_{i-\sigma} b_{j-\sigma} + \mu \sum_{i} \left( \sum_{\sigma} b^{\dagger}_{i\sigma} b_{i\sigma} - 1 \right). \tag{1}$$

The first three terms are just the Heisenberg Hamiltonian $J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$. The last term is introduced to impose the constraint condition $\sum_{\sigma} b^{\dagger}_{i\sigma} b_{i\sigma} = 1$ on the average. $\mu$ is the Lagrange multiplier. Remember that in deriving (1) we have divided the square lattice into two sublattices $A$ and $B$, and used the Schwinger boson representation of the spin operators: $S^z_i = \frac{1}{2}(b^{\dagger}_{i\uparrow} b_{i\uparrow} - b^{\dagger}_{i\downarrow} b_{i\downarrow})$, $S^+_i = b^{\dagger}_{i\uparrow} b_{i\downarrow}$ and $S^-_i = b^{\dagger}_{i\downarrow} b_{i\uparrow}$ for site $(i)$ on the sublattice $A$, and $S^z_j = -\frac{1}{2}(b^{\dagger}_{j\uparrow} b_{j\uparrow} - b^{\dagger}_{j\downarrow} b_{j\downarrow})$, $S^+_j = -b^{\dagger}_{j\downarrow} b_{j\uparrow}$ and $S^-_j = -b^{\dagger}_{j\uparrow} b_{j\downarrow}$ for site (j) on $B$. In the mean field approximation, Hamiltonian (1) is reduced in the **k**-space to the form [13]

$$\mathscr{H} = C + \sum_{\mathbf{k}\sigma}{}' \lambda (b^{A\dagger}_{\mathbf{k}\sigma} b^{A}_{\mathbf{k}\sigma} + b^{B\dagger}_{\mathbf{k}\sigma} b^{B}_{\mathbf{k}\sigma}) - 2J \sum_{\mathbf{k}\sigma}{}' (\rho^{*}_{\sigma} b^{A\dagger}_{\mathbf{k}\sigma} b^{A}_{\mathbf{k}-\sigma} + \rho_{\sigma} b^{B\dagger}_{\mathbf{k}\sigma} b^{B}_{\mathbf{k}-\sigma}) - 2JQ \sum_{\mathbf{k}\sigma}{}' \gamma_{\mathbf{k}} (b^{B\dagger}_{-\mathbf{k}\sigma} B^{A\dagger}_{\mathbf{k}\sigma} + b^{A}_{\mathbf{k}\sigma} b^{B}_{-\mathbf{k}\sigma}), \tag{2}$$

in which $\lambda=\mu-J, C=-N\lambda+NJQ^2+NJ\sum_\sigma \rho_\sigma^* \rho_\sigma$ and $\gamma_{\mathbf{k}}=\frac{1}{2}(\cos \mathbf{k}_x a+\cos \mathbf{k}_y a)$. $N$ is the number of the lattice sites. The prime on the summation means that the sum of $\mathbf{k}$ runs over the first magnetic Brillouin zone. The last term of (2) is arisen from the anomalous mean field decomposition of the 4-boson terms in the Hamiltonian (1), and the order parameter $Q$ is defined by $Q=\sum_\sigma \langle b_{i\sigma} b_{i+\hat{\eta}\sigma}\rangle$ with $\hat{\eta}=\hat{\mathbf{x}}, \hat{\mathbf{y}}$. Differing from Sarker et al., we also take the normal mean field decompositions into account. One of these is just that has been considered in the work of Yoshioka. It is the Hartree term decomposed from the second term of (1). This term together with the last one of (1) gives the second term of the mean field Hamiltonian (2) (and also the constant $\frac{1}{2}NJ-N\mu$). There also exists another Hartree term, decomposed from the third term of (1) which reads

$$-\tfrac{1}{2}J\sum_{\langle ij\rangle}\sum_\sigma (\langle b_{j\sigma}^\dagger b_{j-\sigma}\rangle b_{i\sigma}^\dagger b_{i-\sigma} + b_{j\sigma}^\dagger b_{j-\sigma}\langle b_{i\sigma}^\dagger b_{i-\sigma}\rangle - \langle b_{j\sigma}^\dagger b_{j-\sigma}\rangle\langle b_{i\sigma}^\dagger b_{i-\sigma}\rangle). \quad (3)$$

Transforming these terms into the $\mathbf{k}$-space, one obtains the third term of (2) (and a constant $-2NJ\rho_\sigma^*\rho_\sigma$), in which $\rho_\sigma=\langle b_{i\sigma}^\dagger b_{i-\sigma}\rangle=\frac{2}{N}\sum_{\mathbf{k}}' \langle b_{\mathbf{k}\sigma}^{A\dagger} b_{\mathbf{k}-\sigma}^{A}\rangle$ and $\rho_\sigma^*=\langle b_{j\sigma}^\dagger b_{j-\sigma}\rangle=\frac{2}{N}\sum_{\mathbf{k}}' \langle b_{\mathbf{k}\sigma}^{B\dagger} b_{\mathbf{k}-\sigma}^{B}\rangle$. In the paper [12], the Hartree term (3) is thrown away from beginning. This however is inconsistent as the values of $\langle b_{i\sigma}^\dagger b_{i-\sigma}\rangle$ and $\langle b_{j\sigma}^\dagger b_{j-\sigma}\rangle$ predicted by the theory are finite in the magnetic long range order regime. So it is important to include (3) in the Hamiltonian (2) in order to formulate a consistent mean field theory.

We know that the rotational invariant property of the Hamiltonian is not broken as the spin operators are represented by Schwinger bosons. The long range magnetic ordering is identified with the Bose condensation of the Schwinger bosons and the magnetic moment is ordered in the direction transverse to the $z$-axis [11]. In other words, in the magnetic ordering regime, $\langle S_i^-\rangle$ (and also $\langle S_i^-\rangle$, $\langle S_j^+\rangle$ and $\langle S_j^-\rangle$) is finite and so the order parameter $\rho_\sigma$ (and $\rho_\sigma^*$) does not equal to zero. There is no difficulty to prove that $\rho_\sigma$ can be expressed in terms of the magnetization $\rho$ (in unit of $g\mu_B$) and the angle $\phi$, specified the direction of the sublattice magnetization, through the relation $\rho_\sigma=\rho e^{i\sigma\phi}$. Here $\sigma=1$ $(-1)$ for $S^z=\frac{1}{2}(-\frac{1}{2})$. Let us go back to (3) and re-express it in terms of the spin operator, we see that the Hartree potential $2J\rho_\sigma$ is nothing but the Weiss molecular field. So in our mean field Hamiltonian (2), there exist a term characterizing the antiferromagnetic correlation, and also a term characterizing the nearest neighborhood interaction (Weiss molecular field).

In the disordered regime, only short range order exists. The direction of the local magnetic moment varies with the lattice site. Its average should be zero. So in the disordered regime, $\rho_\sigma=0$. In this case, our mean field Hamiltonian (2) reduces to that of Sarker et al. [11] except that the lagrange multiplier $\mu$ in the later is replaced by its renormalized value $\lambda=\mu-J$. We conclude that when $T>0$ K, AA theory of the $2D$ antiferromagnet is hold even when the normal contractions of the Schwinger boson is considered in the theory.

When $T=0$ K, the situation is quite different. In this case the magnetic moment appears long-range order, and so $\rho_\sigma\neq 0$. Without losing generality, we choose $\phi=0$. It means that we choose the direction of the magnetization of sublattice $A$ as the $x$-axis. By the well known procedure [14, 11], we obtain the following consistent equations for the parameters $Q$ and $\rho$, and also the constraint condition imposed by the Lagrange multiplier:

$$\rho=\frac{n_0}{N}-\frac{1}{4}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\frac{dk_x dk_y}{(2\pi)^2}(f_{\mathbf{k}}-g_{\mathbf{k}}), \quad (4)$$

$$Q=\frac{2n_0}{N}+\frac{1}{2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\frac{dk_x dk_y}{(2\pi)^2}\gamma_{\mathbf{k}}^2(\eta f_{\mathbf{k}}+g_{\mathbf{k}}), \quad (5)$$

$$1=\frac{n_0}{N}+\frac{1}{4}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\frac{dk_x dk_y}{(2\pi)^2}(f_{\mathbf{k}}+g_{\mathbf{k}}), \quad (6)$$

where $\eta=2JQ/(\lambda+2J\rho)$, $f_{\mathbf{k}}=1/\sqrt{1-\eta^2\gamma_{\mathbf{k}}^2}$ and $g_{\mathbf{k}}=1/\sqrt{1-\gamma_{\mathbf{k}}^2}$. Solving these equations numerically, we obtain $\rho=0.4773$, $n_0/N=0.3903$, $Q=1.2108$, $\lambda=3.3763J$ and $\eta=0.5592$. It is to be noted that the sublattice magnetization $\rho$ is somewhat larger than the accepted value 0.3034 predicated by AA and also the cSWT.

By diagonizing the Hamiltonian (2), we find that there are two branches of the Schwinger-boson excitation spectrum

$$\omega_A(\mathbf{k})=(\lambda-2J\rho)\sqrt{1-\gamma_{\mathbf{k}}^2} \text{ (Acoustic)}, \quad (7)$$

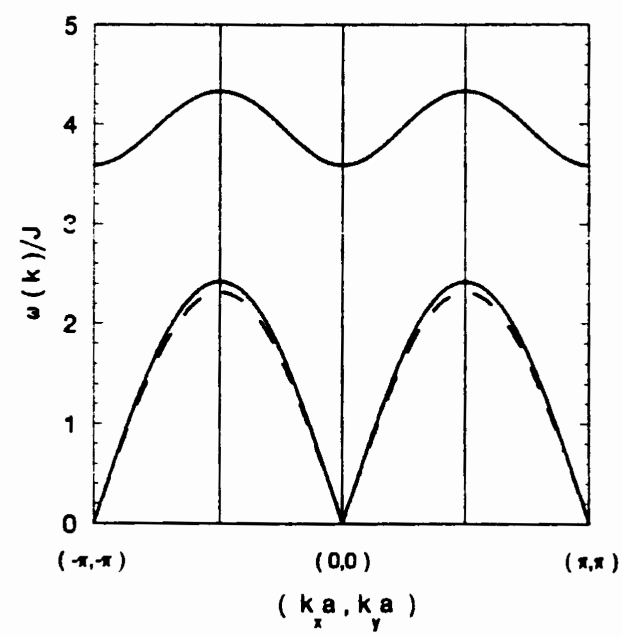


Fig. 1. The Schwinger-boson excitation spectrum along the [1, 1] direction in the $\mathbf{k}$-space. *Solid-line:* our theory; *Dashed line:* AA theory

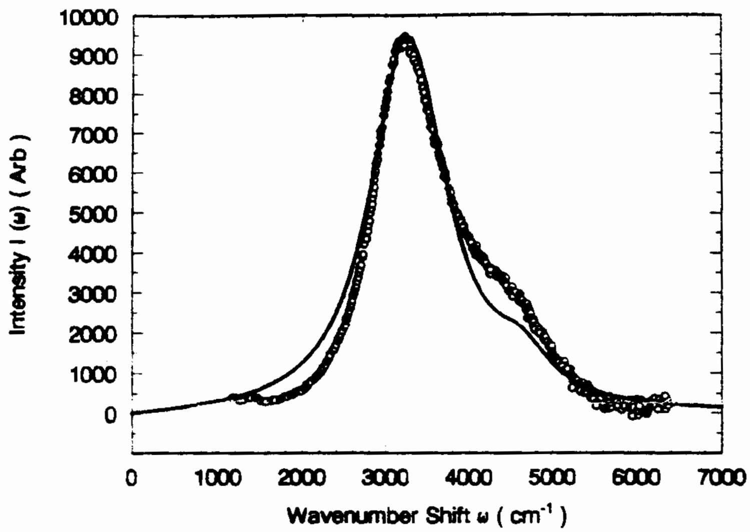


Fig. 2. Raman "two-magnon" spectrum of $La_2CuO_4$. The *circles* are experimental data taken from [7] and the *solid line* is computed from (9) by choosing $\rho=0.3034$, $Q=1.24$, $\eta=0.85$, $J=103.6$ meV and $\Gamma=0.1$

$$\omega_O(\mathbf{k})=(\lambda+2J\rho)\sqrt{1-\eta^2\gamma_{\mathbf{k}}^2}\ \text{(Optical)}. \tag{8}$$

The values of $\rho$, $\lambda$ and $\eta$ are listed below (6). The origin of splitting the degenerate AA excitation spectrums into an acoustic branch and an optical one lies in the presence of the Hartree potential $2J\rho$. The optical branch $\omega_O(\mathbf{k})$ is larger than zero throughout the Brillouin zone. Whereas the acoustic one $\omega_A(\mathbf{k})$ has two zeros at $k=0$ and $\pi$. At such points, the bose condensation occurs. The first term on the right hand side of (4)–(6) are just from the condensation. The spectrum (7) and (8) along the [1, 1] direction are plotted in Fig. 1. For comparison, the Schwinger excitation spectrum predicted by AA is also shown in the same figure by the dashed line. It shows that the acoustic branch of the excitation spectrum $\omega_A(\mathbf{k})$ is essentially the same as that of AA. Whereas the optical branch is the new result outside the AA theory. As shown in the figure there is an energy gap between the two branches of the excitation spectrum. We expect that the values of the parameters such as $\rho$, $\eta$ etc. may suffer more or less modifications if we go beyond the mean field theory and (or) impose strict local constraint condition $\sum_\sigma b_{i\sigma}^\dagger b_{i\sigma}=1$ instead of the average. For example, the value of the sublattice magnetization $\rho$ should be reduced from 0.4773 to 0.3034. And so the energy gap $2JQ(\sqrt{1/\eta^2-1}-1)$ may go out of existence, and even the two excitation branches may overlap in some energy ranges. But we believe that the theoretical prediction about the Schwinger boson excitation spectrum still holds qualitatively.

The present theory provides a natural explanation of the mystery of the Raman "two magnon" scattering from $La_2CuO_4$. Using Green function technique [15] to revise the theory presented in the papers [8, 9], we obtain the following formula for the Raman scattering intensity:

$$I(\varepsilon)\propto-\mathrm{Im}\,\frac{G_0(\varepsilon)}{1+4JG_0(\varepsilon)}, \tag{9}$$

in which

$$G_0(\varepsilon)=\frac{1}{2JQN}\sum_{\mathbf{k}}{}'(2\tilde{\gamma}_{\mathbf{k}})^2\times\left[\frac{1/\eta}{(\varepsilon+2i\Gamma)^2-4(1/\eta^2-\gamma_{\mathbf{k}}^2)}+\frac{1}{(\varepsilon+2i\Gamma)^2-4(1-\gamma_{\mathbf{k}}^2)}\right]. \tag{10}$$

$\Gamma$ is the damping of the boson excitation and $\varepsilon=\omega/(2JQ)$. It is inadequate to compare this theoretical formula directly with the experiment using the mean field value of the parameters $\eta$, $Q$ and $\Gamma$ for the reasons mentioned above. Before we have a more satisfactory theory, we compare it with the experiment in an empirical way. In Fig. 2, the solid line is computed from (9) by choosing $\rho=0.3034$, $Q=1.24$, $\eta=0.85$, $J=103.6$ meV and $\Gamma=0.1$, and the experimental data are taken from Figs. 4–9 of paper [7]. Our theoretical curve shows a long tail and pronounced asymmetry in the shape, especially there is a shoulder located at the same position as the experiment. These interesting features are easily understood if one interprets the Raman spectra roughly as a superposition of two peaks associated with the two branches of the boson excitation separately. As shown in the figure, the agreement between the theory and the experiment is fairly well. This success encourages us to carry out further investigation on the theory of the boson excitation of $2D$ antiferromagnet, and the possibility to explain other optical excitation experiments [16]. This is currently under investigation and the results together with the details of the Raman scattering theory will be published elsewhere.

## References


1. Bedell, K.S., Coffey, P., Meltzer, D.E., Pines, D., Schrieffer, J.R. (eds.): High Temperature Superconductivity. Proceedings of the Los Alamos Symposium. New York: Addison-Wesley 1990
2. Ginsberg, D.M. (ed.): Physical properties of high temperature superconductors. Vol. 1. Singapore: World Scientific 1989
3. Birgeneau, R.J., Shirane, G.: In: [2], p. 151
4. Keffer, F.: Spin wave. In: Handbuch der Physik. Flügge, S. (ed.), Vol. 18, Teil 2. Berlin, Heidelberg, New York: Springer 1966
5. Lyons, K.B., Fleury, P.A., Remeika, J.P., Cooper, A.S., Negran, T.J.: Phys. Rev. **B37**, 2353 (1988)
6. Lyons, K.B., Sulewski, P.E., Fleury, P.A., Carter, H.L., Cooper, A.S., Espinosa, G.P., Fisk, Z., Cheong, S-W.: Phys. Rev. **B39**, 9693 (1989)
7. Marville, L.: Ph.D. thesis, Massachusetts Institute of Technology 1992
8. Parkinson, J.B.: J. Phys. **C2**, 2012 (1969)
9. Elliott, R.J., Thorpe, M.F.: J. Phys. **C2**, 1630 (1969)
10. Arovas, D.P., Auerbach, A.: Phys. Rev. **B38**, 316 (1988)
11. Sarker, S., Jayaprakash, C., Krishnamurthy, H.R., Ma, M.: Phys. Rev. **B40**, 5028 (1989)
12. Yoshioka, D.: J. Phys. Soc. Jpn. **58**, 32 (1989)
13. In the mean field Hamiltonian (2), there are two other terms: $-J\chi \sum'_{\mathbf{k}\sigma} \gamma_{\mathbf{k}} (b^{A+}_{\mathbf{k}\sigma} b^{B}_{\mathbf{k}\sigma} + b^{B+}_{\mathbf{k}\sigma} b^{A}_{\mathbf{k}\sigma})$ and $-iJ\tilde{\chi} \sum'_{\mathbf{k}\sigma} \tilde{\gamma}_{\mathbf{k}} \sigma (b^{A+}_{\mathbf{k}\sigma} b^{B}_{\mathbf{k}-\sigma} + b^{B+}_{k-\sigma} b^{A}_{\mathbf{k}\sigma})$ in which $\chi = \sum_{\sigma} \langle b^{+}_{i\sigma} b_{i+\eta\sigma} \rangle$, $\tilde{\chi} = \sum_{\sigma} \sigma \langle b^{+}_{i\sigma} b_{i+\eta-\sigma} \rangle$ and $\tilde{\gamma}_{\mathbf{k}} = \frac{1}{2}(\sin k_x a + \sin k_y a)$. Our numerical computation shows that $\tilde{\chi}$ is always zero, and $\chi$ can be either zero or nonzero. However, it is only when $\chi = 0$ that there are two points $k = 0$ and $\pi$ at which the bose condensation occurs. So for the theory of antiferromagnet, we choose the solution $\chi = 0$
14. Kane, C.L., Lee, P.A., Ng, T.K., Chakraborty, B., Read, N.: Phys. Rev. **B41**, 2653 (1990)
15. Abrikosov, A.A., Gorkov, L.P., Dzyaloshinski, I.E.: Methods of quantum field theory in statistical physics. Englewood Cliffs, N.J.: Prentice-Hall
16. Thomas, G.A., Rapkine, D.H., Cooper, S.L., Cheong, S-W., Cooper, A.S., Schneemeyer, L.F., Waszczak, J.V.: Phys. Rev. **B45**, 2474 (1992)