The random-phase-approximation in the weak coupling regime of the square lattice half-filled Hubbard model

Peter Kopietz

Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, W-7000 Stuttgart 80, Federal Republic of Germany

We re-examine the random-phase approximation (RPA) in the antiferromagnetic spin-density-wave state of the half-filled square lattice repulsive Hubbard model. It is shown that for $U/t \ll 1$ the RPA yields a vanishing spin-wave velocity, $\hbar c \sim 2\pi^{-1/2} t (U/t)^{1/4}$, a diverging uniform transverse susceptibility, $\chi_\perp \sim (2\pi t)^{-1} (U/t)^{-1/2}$, and a constant spin stiffness, $\rho_s \sim 2\pi^{-2} t$. The behavior of ρ_s shows that the RPA cannot be correct in the weak coupling regime, because ρ_s should vanish in the limit $U/t \to 0$. We give a formally exact expression for ρ_s and identify the term which is neglected within the RPA.

One of the most popular theoretical models, that has been used many times to explain the unusual properties of the high temperature superconductors, is the two dimensional Hubbard model on a square lattice, with Hamiltonian given by

$$\mathcal{H} = -t \sum_{\substack{\langle \mathbf{r}, \mathbf{r}' \rangle \\ \sigma = \uparrow, \downarrow}} [c^\dagger_{\mathbf{r}\sigma} c_{\mathbf{r}'\sigma} + c^\dagger_{\mathbf{r}'\sigma} c_{\mathbf{r}\sigma}] + U \sum_{\mathbf{r}} c^\dagger_{\mathbf{r}\uparrow} c_{\mathbf{r}\uparrow} c^\dagger_{\mathbf{r}\downarrow} c_{\mathbf{r}\downarrow}. \quad (1)$$

Here $\mathbf{r}$ labels the N sites of a square lattice, the first sum is over the $2N$ nearest neighbor bonds, and $c_{\mathbf{r}\sigma}$ is the destruction operator for a spin-σ electron at site $\mathbf{r}$. In the present paper we shall only consider the case of half filling. Even then the ground state is not exactly known. For $U/t \gg 1$, (1) reduces to the Hamiltonian of the spin $S = 1/2$ square lattice Heisenberg antiferromagnet with an exchange coupling of $J = 4t^2/U$. There is convincing evidence [1] that the ground state of this model has antiferromagnetic long-range order (LRO), although a rigorous proof is still lacking. The most naive guess is then that the antiferromagnetic LRO is maintained in the half-filled Hubbard model for any $U/t > 0$, and vanishes only at $U/t = 0$. This guess is the starting point of the random-phase-approximation (RPA), where the spectrum of the collective spin-wave modes is approximately obtained by summing an infinite set of se-

lected ladder diagrams describing particle-hole excitations around a mean-field ground state, which is assumed be an antiferromagnetic spin-density wave [2, 3]. Note that even for arbitrarily small U/t it is necessary to sum an infinite number of terms in the perturbative expansion, because the Goldstone-poles in the order parameter correlation function, which by spin-rotational symmetry are guaranteed to exist for any $U/t > 0$, cannot be obtained at any finite order in perturbation theory.

In spite of the fact that the RPA is an expansion around the weak coupling limit, extrapolation of the RPA result for the spin-wave spectrum maps for $U/t \to \infty$ onto the well known spin-wave spectrum of the Heisenberg model. The naive expectation is that if RPA is correct at strong coupling, it should work even better at weak coupling, because it is by definition a weak coupling expansion. This has led many physicists to the believe that the ground state of the half filled square lattice Hubbard model has LRO for any finite U/t.

In two recent papers [4, 5] the present author has developed a functional integral approach for the Hubbard model, which takes into account the $SU(2)$-symmetry and the fluctuations of the Goldstone modes in a quite elegant way. In contrast to the RPA, this approach is a systematic expansion around the strong coupling regime. Quite surprisingly, and in apparent contradiction with the RPA-results, it was found that an extrapolation of the strong coupling theory to the weak coupling regime was not possible, and that due to the quantum fluctuations of the Goldstone modes the antiferromagnetic spin-density-wave should become unstable at $U/t = O(1)$. If two approximate calculations give different results, at least one of them is necessarily wrong. In the present paper we show that the RPA cannot be correct for $U/t \ll 1$. Let us briefly rederive the RPA-results in the weak coupling regime with a minimum of algebra.

The object of interest is the transverse susceptibility for the staggered magnetization, $\chi_{st}(\mathbf{k}, z)$. For convenience, we shall use the Matsubara technique, and calculate

$$\chi_{st}(\mathbf{k}, i\omega_n) = \sum_{\mathbf{r}} \int_0^{\frac{1}{T}} d\tau \, e^{i\omega_n\tau - i(\mathbf{k}+\mathbf{Q})\cdot\mathbf{r}} \frac{1}{Z}$$
$$\cdot \mathrm{Tr}\{e^{-(\mathcal{H}-\mu\mathcal{N})/T} \tfrac{1}{2}[S_{\mathbf{r}}^+(\tau) S_0^-(0)$$
$$+ S_{\mathbf{r}}^-(\tau) S_0^+(0)]\} \qquad (2)$$

where T is the temperature, $\omega_n = 2\pi n T$, μ is the chemical potential, Z is the grand canonical partition function, $S_{\mathbf{r}}(\tau) = e^{(\mathcal{H}-\mu\mathcal{N})\tau} S_{\mathbf{r}}(0) e^{-(\mathcal{H}-\mu\mathcal{N})\tau}$, and $\mathcal{N}$ is the particle number operator. The antiferromagnetic ordering wave vector is $\mathbf{Q} = [\pi, \pi]$. (All lengths are measured in units of the lattice spacing in the present work.) In a spherical basis the components of the spin operator $S_{\mathbf{r}}$ are given by

$$S_{\mathbf{r}}^+ = (S_{\mathbf{r}}^-)^\dagger = c_{\mathbf{r}\uparrow}^\dagger c_{\mathbf{r}\downarrow} \text{ and } S_{\mathbf{r}}^z = \tfrac{1}{2}[c_{\mathbf{r}\uparrow}^\dagger c_{\mathbf{r}\uparrow} - c_{\mathbf{r}\downarrow}^\dagger c_{\mathbf{r}\downarrow}].$$

Let us now assume that even for arbitrarily small $U/t > 0$ the ground state has antiferromagnetic LRO. Then the

now straight forward to evaluate the expectation values in (2) and (3) with the eigenstates of the Hartree-Fock Hamiltonian. For $T \to 0$ one obtains from (3)

$$\frac{1}{U} = \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{E_{\mathbf{k}}}, \qquad (8)$$

and for the susceptibility

$$\chi_{st}^{HF}(\mathbf{k}, i\omega_n) = \frac{1}{N} \sum_{\mathbf{q}} (v_{\mathbf{q}} v_{\mathbf{q}+\mathbf{k}} + u_{\mathbf{q}} u_{\mathbf{q}+\mathbf{k}})^2$$
$$\cdot \left[\frac{1}{E_{\mathbf{q}} + E_{\mathbf{q}+\mathbf{k}} - i\omega_n} + \frac{1}{E_{\mathbf{q}} + E_{\mathbf{q}+\mathbf{k}} + i\omega_n} \right]. \qquad (9)$$

Using (8) and the fact that $v_{\mathbf{q}}^2 + u_{\mathbf{q}}^2 = 1$, it is easy to see that $\chi_{st}^{HF}(0,0) = 1/U$. If we then attempt a perturbative expansion in powers of the interaction, we encounter a divergence even for infinitesimal $U/t > 0$. A closer inspection of the structure of the higher order terms shows

coupling limit [7]. Thus, for $U/t \ll 1$ the complications arising from matrix-formalisms [2, 3] can be avoided.

At the first sight (12), (13) and (15) seem to imply the spin-wave velocity is of order t at weak coupling, but this is incorrect. To evaluate the integrals, it is convenient to introduce the auxiliary functions

$$\rho(\gamma) = \int \frac{d^2 q}{2\pi^2} \delta(\gamma - \gamma_\mathbf{q}) = \frac{4}{\pi^2} K(1 - \gamma^2) \qquad (17)$$

$$w(\gamma) = \int \frac{d^2 q}{2\pi^2} \delta(\gamma - \gamma_\mathbf{q}) \frac{\sin^2 q_x + \sin^2 q_y}{2}$$

$$= \frac{8}{\pi^2} [E(1 - \gamma^2) - \gamma^2 K(1 - \gamma^2)], \qquad (18)$$

where $K(x)$ and $E(x)$ are the usual complete elliptic integrals. Note that only $\rho(\gamma)$ has a logarithmic singularity at the zone boundary $\gamma = 0$. Defining the dimensionless parameter $\lambda = 4t/\Delta$, we obtain from (12), (13), (15) and (16) after some simple rescalings

$$\hbar c = 2\sqrt{2} t \sqrt{\frac{f(\lambda)}{g(\lambda)}}, \quad \chi_\perp = \frac{\lambda}{16t} g(\lambda), \quad \rho_s = \frac{t}{2} \lambda \bar{f}(\lambda), \quad (19)$$

with

$$f(\lambda) = \frac{4}{\pi^2} \int_0^1 d\gamma \left[\frac{E(1-\gamma^2)}{(1+\lambda^2 \gamma^2)^{3/2}} \left[\frac{3}{1+\lambda^2 \gamma^2} - 1 \right] \right.$$

$$\left. - 3\gamma^2 \frac{K(1-\gamma^2)}{(1+\lambda^2 \gamma^2)^{5/2}} \right] \qquad (20)$$

$$g(\lambda) = \frac{4}{\pi^2} \int_0^1 d\gamma \frac{K(1-\gamma^2)}{(1+\lambda^2 \gamma^2)^{3/2}}. \qquad (21)$$

For $U/t \ll 1$ the solution of (8) is given by $M_{st} = (4t/U)e^{-2\pi\sqrt{t/U}}$. Then λ becomes exponentially large, $\lambda \sim e^{2\pi\sqrt{t/U}}$. For large λ we have $f(\lambda) \sim 4\pi^{-2}\lambda^{-1}$ and $g(\lambda) \sim 4\pi^{-2}(\ln \lambda) \lambda^{-1}$, so that we finally obtain from (19) for $U/t \ll 1$

$$\hbar c = \frac{2t}{\sqrt{\pi}} \left(\frac{U}{t}\right)^{1/4}, \quad \chi_\perp = \frac{1}{2\pi t} \left(\frac{U}{t}\right)^{-1/2}, \quad \rho_s = \frac{2t}{\pi^2}. \quad (22)$$

In the weak coupling regime spin-waves are defined only at long wavelengths and low energies, where the vicinity to the pole in (10) leads to a large susceptibility. From (11) we see that the pole becomes dominant if $UA\omega_n^2 \ll 1$ and $UBk^2 \ll 1$. For $U/t \ll 1$ we have

$$UA = U\Delta^{-3} g(\lambda)/8 \sim (U/t)^{1/2}/(4\pi\Delta^2), \quad \text{and}$$
$$UB = U t^2 \Delta^{-3} f(\lambda)/2 \sim U t/(2\pi^2 \Delta^2).$$

It follows that in the weak coupling regime the RPA-spin-waves are well defined if

$$|\omega_n| \ll (4\pi)^{1/2} \Delta \left(\frac{U}{t}\right)^{-1/4}, \quad \hbar c k \ll (8\pi)^{1/2} \Delta \left(\frac{U}{t}\right)^{-1/4}. \quad (23)$$
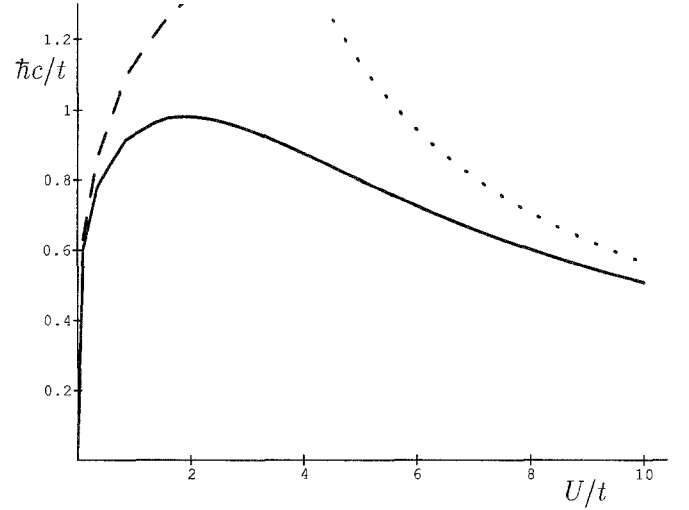

Fig. 1. RPA-result for the spin-wave velocity (solid line). The dashed line is the weak coupling behavior (see (19)), and the dotted line is the strong coupling result $\hbar c = \sqrt{2} J$

Note that the cutoff energy is large compared with Δ. We conclude that within RPA the spin-wave velocity vanishes in the weak coupling limit as $(U/t)^{1/4}$, while $\chi_\perp$ diverges as $(U/t)^{-1/2}$. We disagree in this point with [2]. Note, however, that the maximum at $U/t \approx 2$ shown in Fig. 3 of [3] (a feature which is missing in Fig. 4 of [2]) signals the beginning of the weak coupling regime described by (22). Thus, our analytical result is in agreement with the numerical evaluation of [3]. In Fig. 1 we show the correct RPA-result for the spin-wave velocity, using the results of [3] in the strong coupling regime [7].

The expression for ρ_s in (22) cannot be correct, because the spin stiffness has to vanish in the limit of vanishing M_{st}. To understand why the RPA is not sufficient to describe the weak coupling regime, it is necessary to recall the microscopic definition of the spin stiffness in a magnetially ordered system [8]. (In a system without magnetic order, such as the square lattice Hubbard model at any $T \neq 0$, we have exactly $\rho_s = 0$.) Suppose we impose a slow twist of wavelength $2\pi/Q$ in the direction of $\mathbf{M}_{st}$. Then the energy $F(Q)$ in the presence of the twist increases. The spin stiffness measures the curvature of this increase at $Q = 0$,

$$\rho_s = \lim_{Q \to 0} \lim_{N \to \infty} \frac{1}{N} \frac{\partial^2 F(Q)}{\partial Q^2}. \qquad (24)$$

In [5] we have shown that if one calculates $F(Q)$ at the level of the Hartree-Fock approximation, one obtains from (24)

$$\rho_s^{HF} = \frac{t}{2} \lambda \bar{f}(\lambda), \qquad (25)$$

with

$$\bar{f}(\lambda) = \frac{4}{\pi^2} \int_0^1 d\gamma \frac{\gamma^2 K(1-\gamma^2)}{(1+\lambda^2 \gamma^2)^{1/2}}. \qquad (26)$$

Obviously, (25) agrees with the RPA-result in (19) provided $f(\lambda) = \tilde{f}(\lambda)$. Although (20) and (26) look rather different, they are indeed two equivalent integral representations of the same function. To proof this, it is sufficient to show that in the complex λ^2-plane both functions are for Re $\lambda^2 > -1$ free of singularities and have the same power expansion with finite radius of convergence around the origin [9]. Elementary complex function theory implies then that these functions must be identical. As a byproduct, we obtain a much simpler represen-

result in the weak coupling regime. Only in the strong coupling regime (29) is a small correction to ρ_s^{dia}, corresponding to higher orders in $1/(2S)$ in spin-wave theory [5]. For $0 < U/t \ll 1$ there are two possibilities: The first is that the cancellation between ρ_s^{dia} and ρ_s^{para} is not perfect, so that ρ_s is finite, but certainly $\rho_s^{\text{dia}} + \rho_s^{\text{para}} \ll \rho_s^{\text{dia}}$. Intuitively, we expect that the exponentially small magnetization is accompanied by an exponentially small spin stiffness, so that ρ_s should be proportional to some power of Δ. The second possibility is that the spin stiffness re-

$$B = \left(\frac{t}{\Delta}\right)^2 \frac{2}{N} \sum_{\mathbf{q}} \frac{\gamma_{\mathbf{q}}^2}{E_{\mathbf{q}}}. \tag{27}$$

Unlike (13) this representation manifestly shows that $B > 0$.

From the agreement between ρ_s^{HF} and the RPA-result for ρ_s in (19) we conclude that within RPA one obtains the spin stiffness at the mean-field level. To see more

LRO for small U/t. This is the scenario discussed in [5].

In summary, we have shown that the random-phase approximation in the square-lattice half-filled Hubbard model yields unphysical results for $U/t \ll 1$. We have here the peculiar situation that a weak coupling expansion works only in the strong coupling limit! More work is required to examine the weak coupling regime beyond the RPA-level. It has been shown in the present work