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Antiferromagnetism and single-particle properties in the two-dimensional half-filled Hubbard model: Slater *vs.* Mott-Heisenberg

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Abstract. – We study antiferromagnetism and single-particle properties in the two-dimensional half-filled Hubbard model at low temperature. Collective spin fluctuations are governed by a non-linear sigma model that we derive from the Hubbard model for any value of the Coulomb repulsion. As the Coulomb repulsion increases, the ground state progressively evolves from a Slater to a Mott-Heisenberg antiferromagnet. At finite temperature, we find a metal-insulator transition between a pseudogap phase at weak coupling and a Mott-Hubbard insulator at strong coupling.

Introduction. – The Hubbard model [1] and its generalizations play a key role in the description of strongly correlated fermion systems such as high-T_c superconductors, heavy fermions systems, or organic conductors [2]. Despite its simplicity (the model is defined by two parameters, the inter-site hopping amplitude t and the local Coulomb interaction U, and the symmetry of the lattice), exact solutions or well-controlled approximations exist only in a few special cases as in one-dimension (1D) or in the limit of infinite dimension [1].

It is now well established that the ground state of the 2D half-filled Hubbard model on a square lattice has antiferromagnetic (AF) long-range order. The origin of antiferromagnetism is believed to depend on the strength of the Coulomb repulsion. At weak coupling ($U \ll t$), a Fermi surface instability gives rise to an insulating spin-density-wave ground state as first suggested by Slater [3]. In 2D, thermal (classical) fluctuations preclude a finite-temperature transition (Mermin-Wagner theorem) and the phase transition occurs at $T_{\rm N} = 0$. Since the fermion spectral function is gapped at $T = 0$, one expects, from a continuity argument, that it will exhibit a pseudogap at finite temperature as a result of strong AF fluctuations [4]. At strong coupling ($U \gg t$), the system becomes a Mott-Hubbard insulator below a temperature of the order of U. The resulting local moments develop AF short-range order at a much smaller temperature ($\sim J = 4t^2/U$), and AF long-range order sets in at $T_{\rm N} = 0$.

Although the Hartree-Fock (HF) theory gives a reasonable description of the AF ground state, it fails in 2D since it predicts AF long-range order. Several alternative approaches, which do satisfy the Mermin-Wagner theorem, have been proposed: Moriya's self-consistent renormalized theory [5], the fluctuation exchange approximation (FLEX) [6], and the two-particle self-consistent approach [4]. However, these approaches are restricted to the weak-to-intermediate coupling regime ($U \sim 4t$). The strong-coupling regime is usually understood from the Heisenberg model for which various methods are available [7].

In this letter, we describe a theoretical approach which provides a unified view of antiferromagnetism and single-particle properties in the 2D half-filled Hubbard model at low temperature (including $T = 0$) and for any value of the Coulomb repulsion. It is based on a non-linear sigma model (NLσM) description of spin fluctuations. Since it takes into account only directional fluctuations of the AF order parameter, it is valid below a crossover temperature $T_{\rm X}$ which marks the onset of AF short-range order.

Besides its validity both at weak and strong coupling, our approach differs from previous weak-coupling theories [4–6] by the fact that it is a low-temperature expansion ($0 \le T \ll T_{\rm X}$). In particular, the fermion spectral function is obtained from a spin-rotation-invariant perturbative expansion around the (gapped) HF ordered state. This should be contrasted with perturbative treatments applied to (gapless) free fermions interacting with soft collective spin fluctuations where no small expansion parameter is available [8]. In ref. [9], one of the present authors reported a calculation of the spectral function in the weak-coupling limit of the Hubbard model using a NLσM description of spin fluctuations. However, the limitations encountered by previous weak-coupling theories could not be fully overcome.

Non-linear sigma model. – The Hubbard model is defined by the Hamiltonian

$$H = -t \sum_{\langle \boldsymbol{r},\boldsymbol{r}'\rangle,\sigma} \left(c^\dagger_{\boldsymbol{r}\sigma} c_{\boldsymbol{r}'\sigma} + \text{h.c.}\right) + U \sum_{\boldsymbol{r}} n_{\boldsymbol{r}\uparrow} n_{\boldsymbol{r}\downarrow}. \tag{1}$$

$c^\dagger_{\boldsymbol{r}\sigma}$ ($c_{\boldsymbol{r}\sigma}$) creates (annihilates) a fermion of spin σ at the lattice site $\boldsymbol{r}$. $n_{\boldsymbol{r}\sigma} = c^\dagger_{\boldsymbol{r}\sigma} c_{\boldsymbol{r}\sigma}$ and $\langle \boldsymbol{r}, \boldsymbol{r}'\rangle$ denotes nearest-neighbor sites. We take the lattice spacing equal to unity and $\hbar = k_{\rm B} = 1$.

We express charge and spin fluctuations in terms of auxiliary fields. For this purpose, we write the interaction term in (1) as $n_{\boldsymbol{r}\uparrow} n_{\boldsymbol{r}\downarrow} = [(c^\dagger_{\boldsymbol{r}} c_{\boldsymbol{r}})^2 - (c^\dagger_{\boldsymbol{r}} \boldsymbol{\sigma} \cdot \boldsymbol{\Omega}_{\boldsymbol{r}} c_{\boldsymbol{r}})^2]/4$, where $\boldsymbol{\Omega}_{\boldsymbol{r}}$ is an arbitrary unit vector [10]. $c_{\boldsymbol{r}} = (c_{\boldsymbol{r}\uparrow}, c_{\boldsymbol{r}\downarrow})^T$ and $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ denotes the Pauli matrices. Spin-rotation invariance is made explicit by averaging the partition function over all directions of $\boldsymbol{\Omega}_{\boldsymbol{r}}$. In a path-integral formalism, $\boldsymbol{\Omega}_{\boldsymbol{r}}$ becomes a time-dependent field. Decoupling the interaction term by means of two real auxiliary fields, Δ_c and Δ_s, the partition function is then given by $Z = \int \mathcal{D}[c^\dagger, c] \int \mathcal{D}[\Delta_c, \Delta_s, \boldsymbol{\Omega}_{\boldsymbol{r}}] e^{-S}$ with the action ($\beta = 1/T$)

$$S = S_0 + \int_0^\beta \mathrm{d}\tau \sum_{\boldsymbol{r}} \left[\frac{\Delta^2_{c\boldsymbol{r}} + \Delta^2_{s\boldsymbol{r}}}{U} - c^\dagger_{\boldsymbol{r}} \left(i\Delta_{c\boldsymbol{r}} + \Delta_{s\boldsymbol{r}} \boldsymbol{\sigma} \cdot \boldsymbol{\Omega}_{\boldsymbol{r}}\right) c_{\boldsymbol{r}}\right], \tag{2}$$

where $c_{\boldsymbol{r}}$, $c^\dagger_{\boldsymbol{r}}$ are Grassmann variables. S_0 is the action in the absence of interaction. Equation (2) defines an "amplitude-direction" representation, where the AF order parameter field is given by $\Delta_{s\boldsymbol{r}} \boldsymbol{\Omega}_{\boldsymbol{r}}$. In the following, charge fluctuations (Δ_c) are considered at the saddle-point (*i.e.* HF) level: $-i\Delta_{c\boldsymbol{r}} = (U/2)\langle c^\dagger_{\boldsymbol{r}} c_{\boldsymbol{r}}\rangle = U/2$. Below the HF transition temperature $T_{\rm N}^{\rm HF}$, the amplitude of the order parameter takes a well-defined value so that we can consider $\Delta_{s\boldsymbol{r}}$ within a saddle-point approximation, *i.e.* $\Delta_{s\boldsymbol{r}} = \Delta_0$, where the fluctuations of Δ_0 are ignored. When $T \ll T_{\rm N}^{\rm HF}$, $\Delta_0 \sim t e^{-2\pi\sqrt{t/U}}$ for $U \ll t$ and tends to $U/2$ for $U \gg t$. Below the crossover temperature $T_{\rm X}$ (to be defined more precisely later) which marks the onset of AF short-range order, the $\boldsymbol{\Omega}_{\boldsymbol{r}}$ field can be parametrized by $\boldsymbol{\Omega}_{\boldsymbol{r}} = (-1)^{\boldsymbol{r}} \boldsymbol{n}_{\boldsymbol{r}} (1 - \boldsymbol{L}^2_{\boldsymbol{r}})^{1/2} + \boldsymbol{L}_{\boldsymbol{r}}$, where the Néel field $\boldsymbol{n}_{\boldsymbol{r}}$ ($|\boldsymbol{n}_{\boldsymbol{r}}| = 1$) is assumed to be slowly varying [11]. The small canting vector $\boldsymbol{L}_{\boldsymbol{r}}$, orthogonal to $\boldsymbol{n}_{\boldsymbol{r}}$, takes account of local ferromagnetic fluctuations. It turns out to be convenient to introduce a pseudo-fermion $\phi_{\boldsymbol{r}\sigma}$ whose spin is quantized along the (fluctuating)

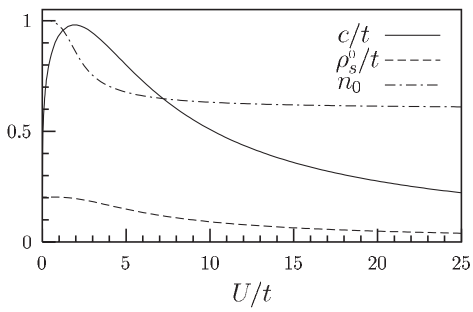

Fig. 1 – Spin-wave velocity c, bare spin stiffness ρ_s^0, and fraction n_0 of condensed bosons at $T = 0$.

Néel field. $\phi_{\boldsymbol{r}} = (\phi_{\boldsymbol{r}\uparrow}, \phi_{\boldsymbol{r}\downarrow})^T$ is defined by $c_{\boldsymbol{r}} = R_{\boldsymbol{r}}\phi_{\boldsymbol{r}}$, where $R_{\boldsymbol{r}}$ is a site- and time-dependent $SU(2)/U(1)$ matrix satisfying $R_{\boldsymbol{r}}\sigma_3 R_{\boldsymbol{r}}^\dagger = \boldsymbol{\sigma}\cdot\boldsymbol{n}_{\boldsymbol{r}}$. The action can then be written as

$$S = \int_0^\beta \mathrm{d}\tau \sum_{\boldsymbol{r}} \phi_{\boldsymbol{r}}^\dagger \left\{ \partial_\tau - A_{0\boldsymbol{r}} - 2t \sum_{\mu=x,y} \cos\left(-i\partial_\mu - A_{\mu\boldsymbol{r}}\right) - \Delta_0 \left[(-1)^{\boldsymbol{r}} \sigma_3 \sqrt{1-\boldsymbol{l}_{\boldsymbol{r}}^2} + \boldsymbol{l}_{\boldsymbol{r}}\cdot\boldsymbol{\sigma} \right] \right\} \phi_{\boldsymbol{r}}, \quad (3)$$

where we have introduced the $SU(2)$ gauge field $A_{0\boldsymbol{r}} = -R_{\boldsymbol{r}}^\dagger \partial_\tau R_{\boldsymbol{r}}$, $A_{\mu\boldsymbol{r}} = iR_{\boldsymbol{r}}^\dagger \partial_\mu R_{\boldsymbol{r}}$ ($\mu = x, y$), and the rotated canting field $\boldsymbol{l}_{\boldsymbol{r}} = \mathcal{R}_{\boldsymbol{r}}^{-1}\boldsymbol{L}_{\boldsymbol{r}}$. Here $\mathcal{R}_{\boldsymbol{r}}$ is the $SO(3)$ element associated to $R_{\boldsymbol{r}}$ which maps $\hat{\boldsymbol{z}}$ onto $\boldsymbol{n}_{\boldsymbol{r}}$. In eq. (3), both $\boldsymbol{l}$ and A_μ are small, since the gauge field is of order $\partial_\mu \boldsymbol{n}$. The effective action of the Néel field is obtained by expanding (3) to second order in these variables and integrating out the fermions and the canting field $\boldsymbol{l}_{\boldsymbol{r}}$. Skipping technical details, we obtain

$$S_{\mathrm{NL}\sigma\mathrm{M}}[\boldsymbol{n}] = \frac{\rho_s^0}{2} \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^2 r \left[\frac{(\partial_\tau \boldsymbol{n}_{\boldsymbol{r}})^2}{c^2} + (\boldsymbol{\nabla}\boldsymbol{n}_{\boldsymbol{r}})^2 \right], \quad (4)$$

where we have taken the continuum limit in real space. The bare spin stiffness ρ_s^0 and the spin-wave velocity c are given by $\rho_s^0 = \epsilon_c/8$ and $c^2 = (\epsilon_c/2)(\chi_\perp^{-1} - U/2)$, where ϵ_c is the absolute value of the (negative) kinetic energy per site and $\chi_\perp$ the transverse spin susceptibility in the HF ground state (fig. 1). In the weak-coupling limit, AF short-range order cannot be defined at length scales smaller than $\xi_0 \sim t/\Delta_0$, which corresponds to the size of bound particle-hole pairs in the HF ground state. Thus eq. (4) should be supplemented with a cutoff $\Lambda \sim \min(1, \xi_0^{-1})$ in momentum space. The NLσM (4) was first obtained by Schulz [12]. In the limit $U \gg t$, it reproduces the result obtained from the Heisenberg model with an exchange coupling $J = 4t^2/U$ [7].

Magnetic phase diagram. – We solve the NLσM within the CP^1 representation, where the Néel field is expressed in terms of two Schwinger bosons: $\boldsymbol{n}_{\boldsymbol{r}} = z_{\boldsymbol{r}}^\dagger \boldsymbol{\sigma} z_{\boldsymbol{r}}$ ($z_{\boldsymbol{r}} = (z_{\boldsymbol{r}\uparrow}, z_{\boldsymbol{r}\downarrow})^T$) with $z_{\boldsymbol{r}}^\dagger z_{\boldsymbol{r}} = 1$. When the CP^1 representation is generalized to the CP^{N-1} representation by introducing N bosons $z_{\boldsymbol{r}\sigma}$ ($\sigma = 1, \dots, N$), the NLσM can be solved exactly by a saddle-point approximation in the $N \to \infty$ limit [7]. At zero temperature, there is a quantum critical point at $g = g_\mathrm{c} = 4\pi/\Lambda$ between a phase with AF long-range order and a (quantum) disordered phase. $g = c/\rho_s^0$ is the coupling constant of the NLσM. In the ordered phase ($g < g_\mathrm{c}$), a fraction $n_0 = 1 - g/g_\mathrm{c}$ ($0 \le n_0 \le 1$) of the bosons condenses in the mode $\boldsymbol{q} = 0$. n_0 determines the mean value of the Néel field: $|\langle \boldsymbol{n}_{\boldsymbol{r}} \rangle| = n_0$. We find that there is AF long-range order for any value of the Coulomb repulsion in the ground state of the 2D half-filled Hubbard model. At weak coupling, $1 - n_0 = g/g_\mathrm{c} \sim e^{-2\pi\sqrt{t/U}}$ is exponentially small. By an appropriate choice of the cutoff Λ, we reproduce the result $n_0 \simeq 0.6$ for $U \gg t$ as obtained from the

2D Heisenberg model on a square lattice [13] (fig. 1). At finite temperature, the AF long-range order is suppressed ($n_0 = 0$). However, the AF correlation length remains exponentially large: $\xi \sim (c/T)e^{2\pi\rho_s/T}$, where $\rho_s = \rho_s^0(1 - g/g_c)$ is the zero temperature spin stiffness. This regime, which is dominated by classical (thermal) fluctuations (since $c/\xi \ll T$), is known as the renormalized classical regime. The NLσM description is valid for $T < T_X$ when amplitude fluctuations of the AF order parameter are frozen and the assumption of AF short-range order holds (*i.e.* $\xi \gg \Lambda^{-1}$). At weak coupling $T_X \sim T_N^{HF}$, while $T_X \sim J$ at strong coupling. The phase diagram is shown in fig. 2. Above T_N^{HF}, spin fluctuations are not important and we expect a Fermi-liquid (FL) behavior. Between T_N^{HF} and T_X (a regime which exists only in the strong-coupling limit), local moments form ($\xi_0 \sim 1$) but with no AF short-range order (Curie spins: $\xi \sim 1$). Below T_X, the system enters a renormalized classical regime of spin fluctuations where the AF correlation length becomes exponentially large. AF long-range order sets in at $T_N = 0$. Although there is a smooth evolution of the magnetic properties as a function of U, the physics is quite different for $U \ll t$ and $U \gg t$. This is shown below by discussing the fermion spectral function. The main conclusions are summarized in fig. 2.

Fermion spectral function. – Now we consider the effect of long-wavelength spin fluctuations on the fermion spectral function. The fermion Green's function $\mathcal{G}(\boldsymbol{r},\tau;\boldsymbol{r}',\tau') = -\langle c_{\boldsymbol{r}}(\tau)c^\dagger_{\boldsymbol{r}'}(\tau')\rangle$, written here as a 2×2 matrix in spin space, is computed using $c_{\boldsymbol{r}} = R_{\boldsymbol{r}}\phi_{\boldsymbol{r}}$ with $(R_{\boldsymbol{r}})_{\uparrow\uparrow} = (R_{\boldsymbol{r}})^*_{\downarrow\downarrow} = z_{\boldsymbol{r}\uparrow}$ and $(R_{\boldsymbol{r}})_{\downarrow\uparrow} = -(R_{\boldsymbol{r}})^*_{\uparrow\downarrow} = z_{\boldsymbol{r}\downarrow}$. Integrating first the pseudo-fermions and the canting field $\boldsymbol{L}_{\boldsymbol{r}}$, we can write the Green's function as

$$\mathcal{G}(1,2) = \frac{1}{Z}\int \mathcal{D}[z]e^{-S_{\mathrm{NL}\sigma\mathrm{M}}[z]}R_1\mathcal{G}(1,2\mid z)R_2^\dagger, \tag{5}$$

where we use the shorthand notation $i \equiv (\boldsymbol{r}_i,\tau_i)$. $\mathcal{G}(1,2\mid z)$ is the pseudo-fermion propagator calculated for a given configuration of the bosonic field z. The action (3), when expanded in powers of A_μ and $\boldsymbol{L}_{\boldsymbol{r}}$, can be written as $S_{\mathrm{HF}}[\phi] + S'[z,\phi,\boldsymbol{L}]$. It describes HF pseudo-fermions interacting with spin fluctuations via the action S'. Since the HF pseudo-fermions are gapped, we expect a perturbative expansion in S' to be well behaved. To leading order $\mathcal{G}(1,2\mid z) = \mathcal{G}^{\mathrm{HF}}(1,2)$ with $\mathcal{G}^{\mathrm{HF}}$ the HF Green's function. From (5), we then obtain

$$\mathcal{G}_\sigma(\boldsymbol{k},\boldsymbol{k}',\omega) = -\frac{2\delta_{\boldsymbol{k},\boldsymbol{k}'}}{\beta}\sum_{\omega_\nu}\int_{\boldsymbol{q}}\mathcal{G}_\sigma^{\mathrm{HF}}(\boldsymbol{k}-\boldsymbol{q},\boldsymbol{k}-\boldsymbol{q},\omega-\omega_\nu)\overline{\mathcal{D}}(\boldsymbol{q},\omega_\nu) + n_0\mathcal{G}_\sigma^{\mathrm{HF}}(\boldsymbol{k},\boldsymbol{k}',\omega), \tag{6}$$

$$\mathcal{G}_\sigma^{\mathrm{HF}}(\boldsymbol{k},\boldsymbol{k}',\omega) = -\delta_{\boldsymbol{k},\boldsymbol{k}'}\frac{i\omega+\epsilon_{\boldsymbol{k}}}{\omega^2+E_{\boldsymbol{k}}^2} + \delta_{\boldsymbol{k},\boldsymbol{k}'+\boldsymbol{\pi}}\frac{\sigma\Delta}{\omega^2+E_{\boldsymbol{k}}^2}, \quad \bar{\mathcal{D}}(\boldsymbol{q},\omega_\nu) = -\frac{gc/2}{\omega_\nu^2+\omega_{\boldsymbol{q}}^2}, \tag{7}$$

where $\int_{\boldsymbol{q}} \equiv \int_{-\pi}^{\pi}\frac{\mathrm{d}q_x}{2\pi}\int_{-\pi}^{\pi}\frac{\mathrm{d}q_y}{2\pi}$, $\boldsymbol{\pi} = (\pi,\pi)$, and ω (ω_ν) denotes a fermionic (bosonic) Matsubara frequency. $\bar{\mathcal{D}}(\boldsymbol{q},\omega_\nu)$ is the Schwinger boson propagator (for $\boldsymbol{q}\neq 0$) obtained from the saddle-point solution of the NLσM. Here $\omega_{\boldsymbol{q}} = c(\boldsymbol{q}^2 + \xi^{-2}/4)^{1/2}$ and $E_{\boldsymbol{k}} = (\epsilon_{\boldsymbol{k}}^2 + \Delta_0^2)^{1/2}$, with $\epsilon_{\boldsymbol{k}} = -2t(\cos k_x + \cos k_y)$ the energy of the free fermions. At finite temperature, n_0 vanishes so that the fermion Green's function is spin-rotation and translation invariant. From (6), we obtain the spectral function $\mathcal{A}(\boldsymbol{k},\omega) = -\pi^{-1}\,\mathrm{Im}\,\mathcal{G}_\sigma(\boldsymbol{k},\boldsymbol{k},i\omega\to\omega+i0^+)$:

$$\mathcal{A}(\boldsymbol{k},\omega) = \mathcal{A}_{\mathrm{inc}}(\boldsymbol{k},\omega) + n_0\mathcal{A}_{\mathrm{HF}}(\boldsymbol{k},\omega), \tag{8}$$

$$\begin{aligned}\mathcal{A}_{\mathrm{inc}}(\boldsymbol{k},\omega) = \int_{\boldsymbol{q}}\frac{gc}{2\omega_q}\Big\{&\big[n_{\mathrm{B}}(\omega_{\boldsymbol{q}})+n_{\mathrm{F}}(-E_{\boldsymbol{k-q}})\big]\big[u^2_{\boldsymbol{k-q}}\delta(\omega-\omega_{\boldsymbol{q}}-E_{\boldsymbol{k-q}})+v^2_{\boldsymbol{k-q}}\delta(\omega+\omega_{\boldsymbol{q}}+E_{\boldsymbol{k-q}})\big]+\\ &+\big[n_{\mathrm{B}}(\omega_{\boldsymbol{q}})+n_{\mathrm{F}}(E_{\boldsymbol{k-q}})\big]\big[u^2_{\boldsymbol{k-q}}\delta(\omega+\omega_{\boldsymbol{q}}-E_{\boldsymbol{k-q}})+v^2_{\boldsymbol{k-q}}\delta(\omega-\omega_{\boldsymbol{q}}+E_{\boldsymbol{k-q}})\big]\Big\},\end{aligned} \tag{9}$$

where $n_{\mathrm{F}}(\omega)$ and $n_{\mathrm{B}}(\omega)$ are the usual Fermi and Bose occupation numbers and $\mathcal{A}_{\mathrm{HF}}$ the HF spectral function: $\mathcal{A}_{\mathrm{HF}}(\boldsymbol{k},\omega) = u_{\boldsymbol{k}}^2\delta(\omega-E_{\boldsymbol{k}}) + v_{\boldsymbol{k}}^2\delta(\omega+E_{\boldsymbol{k}})$, where $u_{\boldsymbol{k}}^2, v_{\boldsymbol{k}}^2 = \frac{1}{2}(1\pm\frac{\epsilon_{\boldsymbol{k}}}{E_{\boldsymbol{k}}})$.

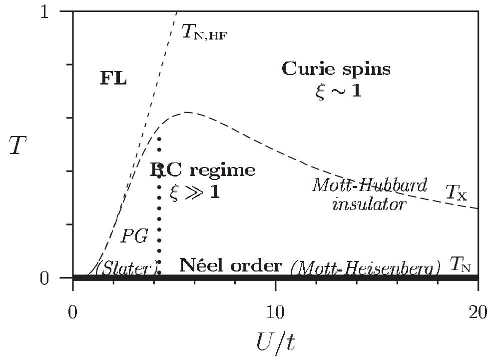

Fig. 2 – Phase diagram of the 2D half-filled Hubbard model. All lines, except $T_{\rm N} = 0$ (thick solid line), are crossover lines. The NLσM description is valid below $T_{\rm X}$. FL: Fermi-liquid phase; PG: pseudogap phase. The vertical dotted line indicates the finite-temperature metal-insulator transition obtained from the criterion $\rho(\omega = 0) = 0$.

The normalization of the spectral function, $\int {\rm d}\omega \mathcal{A}(\boldsymbol{k}, \omega) = 1$, follows from the saddle-point equation of the NLσM.

The spectral function is shown in fig. 3. At weak coupling and zero temperature, our theory describes a Slater antiferromagnet. The AF gap $2\Delta_0 \sim te^{-2\pi\sqrt{t/U}}$ is exponentially small. There are well-defined Bogoliubov quasiparticles (QPs) with energy $\pm E_{\boldsymbol{k}}$, as in the HF theory, but their spectral weight is reduced by a factor n_0 due to quantum spin fluctuations. The remaining weight ($1 - n_0 \sim e^{-2\pi\sqrt{t/U}} \ll 1$) is carried by an incoherent excitation background at higher energy ($|\omega| > E_{\boldsymbol{k}}$). As U increases, the Slater antiferromagnet progressively evolves into a Mott-Heisenberg antiferromagnet with a large AF gap and a significant fraction of spectral weight transferred from the Bogoliubov QPs to the incoherent excitation background. At strong coupling, the AF gap $2\Delta_0 \simeq U$ and $n_0 \simeq 0.6$.

At finite temperature, $\mathcal{A}(\boldsymbol{k}, \omega)$ exhibits two broadened peaks at the HF QP energy $\pm E_{\boldsymbol{k}}$. In the vicinity of the peak at $E_{\boldsymbol{k}}$, the spectral function is well approximated by $\mathcal{A}^{>}_{\rm peak}(\boldsymbol{k}, \omega) = u^2_{\boldsymbol{k}} \frac{g}{4\pi c} n_{\rm B}(|\omega - E_{\boldsymbol{k}}|)$. The peak has a width of the order of the temperature and there-

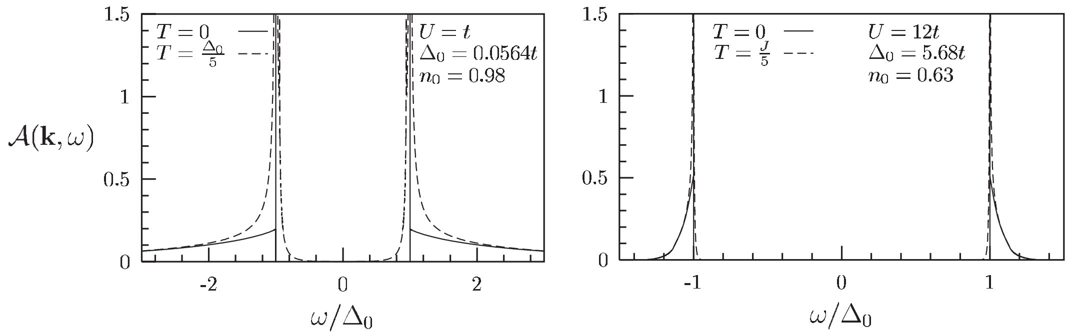

Fig. 3 – Left: spectral function $\mathcal{A}(\boldsymbol{k}, \omega)$ in the weak-coupling limit $U = t$ for $T = 0$ (Slater antiferromagnet) and $T = \Delta_0/5$ (pseudogap phase). Right: spectral function in the strong-coupling regime $U = 12t$ for $T = 0$ (Mott-Heisenberg antiferromagnet) and $T = J/5$ (Mott-Hubbard insulator). $\boldsymbol{k} = (\pi/2, \pi/2)$. For $T = 0$, the vertical lines represent Dirac peaks of weight $n_0/2$. Note the difference in the energy scale, which is fixed by Δ_0, between the two figures.

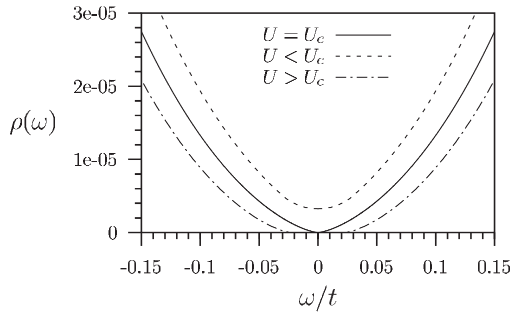

Fig. 4 – Density of states $\rho(\omega)$ at low energy. As the Coulomb repulsion U increases through a critical value $U_\mathrm{c} \simeq 4.25t$, the pseudogap becomes a Mott-Hubbard gap (see the vertical dotted line in fig. 2).

fore corresponds to incoherent excitations. We find that the spectral weight of the peak, $\int \mathrm{d}\omega \mathcal{A}^{>}_{\mathrm{peak}}(\boldsymbol{k}, \omega)$, is temperature independent and equal to $u^2_{\boldsymbol{k}} n_0$, which is nothing else but the Bogoliubov QP weight in the ground state. We conclude that the peak at $E_{\boldsymbol{k}}$ is an incoherent precursor of the zero-temperature Bogoliubov QP peak. As the temperature decreases, it retains its spectral weight but becomes sharper and sharper, and eventually becomes a Dirac peak at $T = 0$. As expected, the weak-coupling pseudogap continuously evolves into the AF gap when $T \to 0$.

Equation (9) shows that the contribution to $\mathcal{A}(\boldsymbol{k}, \omega)$ at low energy involves the Bose occupation number $n_\mathrm{B}(\omega_{\boldsymbol{q}})$. This indicates that the low-energy fermion states ($0 \le |\omega| < E_{\boldsymbol{k}}$) are due to thermal bosons, *i.e.* thermally excited spin fluctuations. A fermion added to the system with momentum $\boldsymbol{k}$ and energy $|\omega| < E_{\boldsymbol{k}}$ can propagate by absorbing a thermal boson of energy $\omega_{\boldsymbol{q}}$ and emitting a pseudo-fermion with energy $E_{\boldsymbol{k}-\boldsymbol{q}} = \omega + \omega_{\boldsymbol{q}}$. The lowest fermion energies are obtained by solving $\omega = E_{\boldsymbol{k}-\boldsymbol{q}} - \omega_{\boldsymbol{q}}$ (or $\omega = -E_{\boldsymbol{k}+\boldsymbol{q}} + \omega_{\boldsymbol{q}}$). In the weak-coupling limit (fig. 3), $\max_{\boldsymbol{q}}(\omega_{\boldsymbol{q}}) = c\Lambda \sim 2\Delta_0$ and $E_{\boldsymbol{k}-\boldsymbol{q}} \sim E_{\boldsymbol{k}}$. Thus, there is spectral weight at zero energy: the spectral function and the density of states exhibit a pseudogap. Nevertheless, the density of states $\rho(\omega) = \int_{\boldsymbol{k}} \mathcal{A}(\boldsymbol{k}, \omega)$ remains exponentially small at low energy: $\rho(\omega) \sim e^{-\Delta_0/T} \cosh(\omega/T)$, $|\omega| \ll \Delta_0$. This result differs from pseudogap theories based on Gaussian spin fluctuations which find a much weaker suppression of the density of states [8]. It bears some similarities with the result obtained by Bartosch and Kopietz for fermions coupled to classical phase fluctuations in incommensurate Peierls chains [14]. In the low-temperature regime dominated by directional fluctuations of the order parameter, the suppression of the density of states at low energy is indeed expected to be exponential. In the strong-coupling limit, since $E_{\boldsymbol{k}} \sim U/2$ and $c\Lambda \sim J \ll U/2$, there is a gap (of order $U/2$) in the spectral function and the density of states. Thermally excited spin fluctuations reduce the zero-temperature AF gap $U/2$ by a small amount of the order of J. The system is a Mott-Hubbard insulator (fig. 2).

We therefore conclude that our approach predicts a finite-temperature metal-insulator transition between a pseudogap phase and a Mott-Hubbard insulator as the strength of the Coulomb interaction increases (fig. 2): at a critical value U_c, the density of states at zero energy $\rho(\omega = 0)$ vanishes and the pseudogap becomes a Mott-Hubbard gap (fig. 4). U_c is obtained by equating the minimum energy Δ_0 of a HF fermion to the maximum energy of a Schwinger boson $\sqrt{m^2 + c^2\Lambda^2}$. For $T \to 0$ the result is $U_\mathrm{c} \simeq 4.25t$. However, being a low-energy theory, the NLσM does not allow us to describe accurately the high-energy Schwinger bosons (with $|\boldsymbol{q}| \sim \Lambda$) and in turn the low-energy fermion excitations. In particular, the critical value of U calculated above and the precise form of the density of states near zero energy, plotted in fig. 4, depend on the cut-off procedure used in the NLσM. Note also that we do not know at which temperature and how the metal-insulator transition ends.

Conclusion. – We have presented a low-temperature approach to the 2D half-filled Hubbard model which allows us to study both collective spin fluctuations and single-particle properties for any value of the Coulomb repulsion U. At zero temperature, it describes the evolution from a Slater to a Mott-Heisenberg antiferromagnet. At finite temperature, it predicts a metal-insulator transition between a pseudogap phase at weak coupling and a Mott-Hubbard insulator at strong coupling. Since the charge auxiliary field Δ_c is considered at the HF level, some aspects of the Mott-Hubbard localization are not taken into account. In particular, at intermediate coupling $U \sim 8t$, we expect both Bogoliubov QP bands (or precursors thereof at finite temperature) and Mott-Hubbard bands in the spectral function [4]. The Mott-Hubbard bands have a purely local origin, independent of the Fermi surface geometry, and should show up at $\omega \sim \pm U/2$ (with $U/2 > \Delta_0$) in the spectral function. Nevertheless, we believe that our theory captures the main features of the physics of the 2D half-filled Hubbard model.

On the basis of a numerical calculation (dynamical cluster approximation), Moukouri and Jarrell have called into question the existence of a Slater mechanism in the 2D Hubbard model [15]. Using the criterion $\rho(\omega = 0) < 10^{-2}/(2t)$ to identify the Mott insulating phase, they concluded that the system is always insulating at low (but finite) temperature even in the weak-coupling limit. From the same criterion ($\rho(\omega = 0) < 10^{-2}/(2t)$), we obtain a similar line in the (U, T)-plane as Moukouri and Jarrell. This shows that the numerical results of ref. [15] are not in contradiction with the existence of a Slater scenario at weak coupling, but reflect the exponential suppression of the density of states due to the presence of a pseudogap.

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