Hole Properties On and Off Magnetization Plateaus in 2D Antiferromagnets

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The phenomenon of magnetization plateaus in antiferromagnets under a magnetic field has always been an important topic in magnetism. We propose to probe the elusive physics of plateaus in 2D by considering a hole-doped antiferromagnet and studying the signatures of magnetization plateaus in terms of the properties of holes, coupled to an effective gauge field generated by the spin sector. The latter mediates interaction between the holes, found to be algebraically decaying and long ranged with both Coulombic and dipolar forms outside the plateau and short ranged (local) inside the plateau. The resulting hole spectral weight is significantly broadened off plateau, while it remains sharply peaked on plateau. We also extend the result obtained for a 1D system where finite hole doping gives rise to a shift in the magnetization value of the plateaus.

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Introduction.—Antiferromagnets under a magnetic field have been known to display magnetization plateaus. The theory of this magnetization plateaus has been an important problem in magnetism and is mainly aimed at providing an explanation of such magnetization plateaus. An even more intriguing question is what happens if we hole dope the antiferromagnet by removing some spins. Hole-doped antiferromagnets have drawn much attention since the discovery of high T_c cuprate superconductivity obtained upon hole doping the parent compound antiferromagnets [1]. Most studies in this context considered Hubbard types of models at a zero field analyzed using slave-particle formalism with an emergent gauge field. The topic constitutes a fundamental problem of importance to all areas of physics: matter-gauge field interaction.

In the area of magnetism itself, antiferromagnets under a magnetic field are widely studied as the field helps select a well-defined ground state, thus allowing for the use of a semiclassical approach, and it gives rise to plateaus. Magnetization plateaus are enhanced by geometric frustration and are also related to exotic states of matter, such as spin liquid states [2]. However, most studies so far have considered undoped antiferromagnets with the hole-doped case not explored much in realistic models [3]. The magnetization plateaus should have immediate consequences on the properties of holes, and this is what we investigate in this work.

The theory of magnetization plateaus, without hole doping, can be relatively well understood with a spin path-integral approach [4]. In one dimension it gives rise to a plateau quantization condition derived based on Lieb-Schultz-Mattis theorem [5,6] as shown first in [7,8]. The presence of holes in 1D can also be treated with bosonization [9–12] and the spin path-integral approach [13,14]. However, generalization of the theory to two and higher dimensions remains a challenge. In this work, we show that one can gain important insights into the physics of a magnetization plateau in higher dimensions by working out the fermion-gauge field theory of a hole-doped antiferromagnet. We demonstrate that the on- and off-plateau states of an antiferromagnet give rise to distinct types of interactions between holes and the resulting spectral function.

Field theory.—We employ a semiclassical path integral theory of a spin system [4] and start with an Euclidean space-time effective action of a 2D antiferromagnet in the presence of holes,

$$S_\phi = \int d^2x \int d\tau \frac{K_\tau}{2}(\partial_\tau \phi)^2 + \frac{K_r}{2}(\nabla\phi)^2 + i\left(\frac{S-m}{a^2}\right)\partial_\tau\phi, \tag{1}$$

$$S_{\bar{\psi},\psi} = \int_{\mathbf{x},\tau} \bar{\psi}(\partial_\tau - ieA_\tau)\psi + \int_{k's} \bar{\psi}_k \epsilon_{k's}(\phi_{k'})\psi_{k''}\delta\left(\sum_{k's}\right), \tag{2}$$

describing low-energy long-distance fluctuations around a classical ground state specified by $\mathbf{S} = S(\sin\theta_0\cos\phi_0, \sin\theta_0\sin\phi_0, \cos\theta_0)$ with spin S and z magnetization $m = S\cos\theta_0$, where ϕ is the phase angle fluctuation field around ϕ_0 [4]. The K_τ, K_r are stiffness coefficients which can be determined from a microscopic spin model [15], giving boson velocity $v_b = \sqrt{K_r/K_\tau}$. The $\bar{\psi}, \psi$ represent the creation and annihilation operator fields of the (spinless) fermionic holes. The $\epsilon_{k's}(\phi_{k'})$ is fermion energy dispersion that couples the holes to the spin sector represented by the ϕ field [16] via the gauge field given as $eA_\mu = e_g\partial_\mu\phi, \mu = \tau, x, y$ with $e \equiv e_g$ the effective gauge charge of the $U(1)$ gauge theory [17]. Our theory will be very generic, but it is aimed to be a paradigm for spin systems well described by Heisenberg model with strong anisotropy and under a magnetic field,

$$H = J\sum_{ij}\mathbf{S}_i \cdot \mathbf{S}_j + D\sum_i (S_i^z)^2 - h\sum_i S_i^z \tag{3}$$

with a classical ground state characterized by $\cos\theta_0 = h/[2S(4J+D)]$ [4], such as those systems with $S = 3/2$ where $1/3$ plateau is expected to occur at large enough D [18].

We will consider a model for holes which, in the realistic case of finite doping, has linear energy dispersion around the Fermi surface. The hole doping itself will give a feedback effect to the spin sector. In such linear fermion dispersion, a sea of occupied negative energy states arises due to linearization and must be removed by applying a projection operator [13,14]; $P_j = 1 - \psi_j^\dagger\psi_j/(2S)$ at each site j on the microscopic lattice model. The doping in turn modifies the plateau quantization condition via normal ordering of the fermion bilinear operator: $\psi_j^\dagger\psi_j = \delta + :\psi_j^\dagger\psi_j:$, where $\delta = \langle\psi_j^\dagger\psi_j\rangle$ is the doping level. We find that with hole doping δ, the plateau occurs at

$$\left(1 - \frac{\delta}{2S}\right)(S \pm m) \in \mathbb{Z} \tag{4}$$

indicating a shift in the magnetization plateau, proportional to doping level δ, compared to the zero doping case, confirming the result in 1D [14].

As was shown in [4], the presence of the Berry phase term plays a crucial role in the large scale physics of the spin sector. If the factor in front of it is an arbitrary real number, field configurations with vortices are forbidden by quantum interference and the Goldstone field ϕ is protected; the system does show long-range order and gapless behavior with no plateau. On the contrary, when the Berry phase factor is an integer, vortex configurations are allowed and, for some values of the spin field stiffness, the system may become disordered and acquire a gap. This is the plateau situation which can be phenomenologically represented by an effective mass term in the Goldstone field, writable as $m_\phi^2\phi^2/2$, into the effective action Eq. (1).

We describe holes in an antiferromagnet as follows. For concreteness, we consider a simple model with holes hopping on a square lattice with nearest-neighbor tight-binding dispersion $\epsilon_k^0 = -2t(\cos k_x + \cos k_y) - \mu$. This gives a Fermi surface with a shape which depends on the chemical potential (and thus filling factor). At chemical potential $\mu = -4t$, we get a Fermi point (corresponding to zero or a thermodynamically small number of hole doping); at $-4t < \mu < 0$, we get a roughly circular Fermi surface that can be described by $k_{Fx}^2 + k_{Fy}^2 = k_F^2 = 4 + \mu/t$; and at half filling $\mu = 0$, we get a square-shaped Fermi surface described by $k_{Fy} = \pm k_{Fx} \pm \pi$.

The fermionic holes will be coupled to a gauge field generated by the spin sector. An effective action for a hole with such a coupling can be derived by considering a tight-binding hopping Hamiltonian [14] with a hopping integral which involves the overlap of the spin coherent states at the neighboring sites between which the hole hops [13], giving the spatial part of the gauge field A_x, A_y, plus applying a projection operator that represents the process of doping holes [14], giving the temporal part of gauge field A_τ. The result is equivalent to a minimal coupling $-i\partial_\mu \to -i\partial_\mu - eA_\mu$ between the spin sector's gauge field and the hole. Considering a nearest-neighbor tight-binding Hamiltonian on a square lattice and applying this minimal coupling to the free hole dispersion ϵ_k^0 gives $\epsilon_{k's}(\phi_{k'}) = -2t(\cos(k_x - ie_g k'_x\phi_{k'}) + \cos(k_y - ie_g k'_y\phi_{k'}))$. Performing Taylor expansion to the two cosine terms around the minimum of the band and doing the Euclidean space-time functional integral, we obtain

$$Z = \int D\bar{\psi}D\psi e^{-\int_k \bar{\psi}_k\epsilon_k^0\psi_k - \delta S_{\bar{\psi},\psi}}, \tag{5}$$

where

$$\delta S_{\bar{\psi},\psi}^{\text{quadratic}} = \int_{k's}\bar{\psi}_{k'''}\psi_{k''}F(k's)G_\phi(k)\bar{\psi}_{k'''''}\psi_{k''''}\delta\left(\sum_{k's}\right), \tag{6}$$

where the function $F(k's)$ and the propagator $G_\phi(k)$ of the Goldstone field are given by

$$F(k's) = e_g^2\left[\frac{1}{4}k_0^2 + t^2(\mathbf{k}\cdot\mathbf{k}''')(\mathbf{k}\cdot\mathbf{k}''''')\right], \tag{7}$$

$$G_\phi^{-1}(k) = \left[\frac{K_\tau}{2}k_0^2 + \frac{K_r}{2}\mathbf{k}^2 + \frac{1}{2}m_\phi^2\right] \tag{8}$$

in Euclidean space-time [19]. We see that the main effects of the spin sector manifest in the form of a 4-fermion interaction term (scattering between two fermions) with a kernel which is massless for a long-range interaction between vortex loops but gapped for a short-range interaction between vortex loops. We note that outside the plateau where $m_\phi \to 0$, as $|\mathbf{k}| \to 0$ the kernel goes as $k_\alpha G_\phi(k)k_\beta \sim 1/K_{\tau,r}$, while in the plateau where $m_\phi \to \infty$, the kernel goes as $k_\alpha G_\phi(k)k_\beta \to 0$. This implies that within the plateau, we have a true short-range interaction between fermionic holes, whereas outside the plateau, we have a nonlocal algebraically decaying interaction between fermionic holes [20]. This 2-fermion scattering action is best illustrated by the Feynman diagram in Fig. 1(a) [21].

An important result of this work is the final form of this 4-fermion interaction term in the out-of-plateau and in-plateau cases, which in Euclidean space-time can be written as

$$\delta S_{\bar{\psi},\psi}^{\text{quadratic}} = \int_{k's}\bar{\psi}_{k'''''}\psi_{k''''}V(k's)\bar{\psi}_{k'''}\psi_{k''}\delta\left(\sum_{k's}\right), \tag{9}$$

where

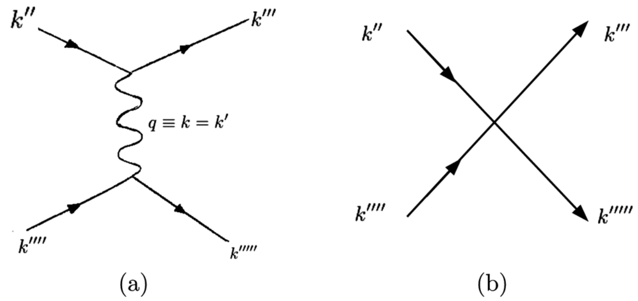

FIG. 1. (a) Feynman diagram of a 2-fermion scattering process mediated by the gauge field. (b) The local interaction vertex counterpart.

$$V^{\text{out-of-plat}}(k's) = \frac{2}{K_s} e_g^2 \frac{[t^2(\mathbf{q}\cdot\mathbf{k}''')(\mathbf{q}\cdot\mathbf{k}''''') + \frac{1}{4}q_0^2]}{q_0^2 + \mathbf{q}^2 + \tilde{m}_s^2}, \quad (10)$$

$$V^{\text{in-plat}}(k's) = \frac{2}{K_s} A e_g^2 [-t^2(\mathbf{k}'''\cdot\mathbf{k}'' - \mathbf{k}''^2)(\mathbf{k}'''''\cdot\mathbf{k}'''' - \mathbf{k}''''^2) - \frac{1}{4}(k_0''''' - k_0'''')(k_0''' - k_0'')] \quad (11)$$

for the out-of-plateau ($m_\phi \to 0$) and in-plateau ($m_\phi \to \infty$) cases represented in Figs. 1(a) and 1(b), respectively. We have rescaled $K_\tau = K_r = K_s$ (equivalent to setting the boson velocity to unity, $v_b = 1$), and the constants are $\tilde{m}_s^2 = m_\phi^2/K_s$ and $A = 1/\tilde{m}_s^2$ [19]. Interestingly, $V^{\text{out-of-plat}}(k's)$ contains an algebraically decaying interaction with a dipolar form in real space in addition to the more conventional density-density interaction term,

$$\delta S_{\text{dip}} = \frac{2}{K_s} t^2 e_g^2 \int_{x_\mu, x'_\mu} \frac{3(\mathbf{d}_1\cdot\Delta\mathbf{r})(\mathbf{d}_2\cdot\Delta\mathbf{r}) - (\mathbf{d}_1\cdot\mathbf{d}_2)|\Delta x|^2}{4\pi|\Delta x|^5}, \quad (12)$$

$$\delta S_{\text{dens}} = -\frac{1}{2K_s} e_g^2 \int_{x_\mu, x'_{\mu'}} \rho(x)\left(\frac{3(\Delta\tau)^2 - |\Delta x|^2}{4\pi|\Delta x|^5}\right)\rho(x'), \quad (13)$$

with dipole moments $\mathbf{d}_1 = [\nabla\bar{\psi}(x)]\psi(x)$, $\mathbf{d}_2 = [\nabla\bar{\psi}(x')]\psi(x')$, $\Delta\tau = \tau' - \tau$, $\Delta\mathbf{r} = \mathbf{x}' - \mathbf{x}$, and $|\Delta x| = |x'_\mu - x_\mu|$, where $x_\mu = (\tau, \mathbf{x})$, $\rho(x) = \bar{\psi}(x)\psi(x)$. In each of Eqs. (10) and (11), the spatial momentum part represents the dipole interaction, whereas the frequency (k_0's) part represents the density-density interaction. Surprising as it is, dipolar interaction intuitively originates from spatial nonuniformity of the hole density distribution, which gives rise to a nonzero effective dipole moment, corresponding to nonzero Fourier wave vectors $\mathbf{k}'s \neq 0$. Such dipolar terms will vanish for a spatially uniform distribution of holes, where only $\mathbf{k}'s = 0$ remains. The presence of both space and time distances in Eqs. (12) and (13), corresponding to the presence of both momentum and frequency dependence in the kernel Eq. (6), reflects the fact that the long-range interaction is not instantaneous as it is mediated by Goldstone bosons with low speed, $v_b \ll c$, in reality. S_{dens} has asymptotic spatial dependence $V(r) \sim 1/r^3$ at large distances and is repulsive [19]. This unexpected result arises from the peculiarity of the gauge field with its origin from the spin sector's physics and its coupling to holes.

Next, we consider finite but low doping levels at $-4t < \mu < 0$, where we have a roughly circular Fermi surface. In this case, we obtain a linearized dispersion $\epsilon_k = 2t[(k_x - k_{xF})\sin k_{xF} + (k_y - k_{yF})\sin k_{yF}]$ where $k_{xF}^2 + k_{yF}^2 = k_F^2 = 4 + \mu/t$ was derived using Taylor series expansion of nearest-neighbor tight-binding energy dispersion $\epsilon_k = -2t(\cos k_x + \cos k_y) - \mu$ around the Fermi surface satisfying $-2t(\cos k_{xF} + \cos k_{yF}) - \mu = 0$ [22]. We obtain 4-fermion interactions and kernels similar to Eqs. (6), (10), and (11) but with the integrals over fermion momenta constrained to be near the Fermi surface only [19]. We observe that the distinction of the physics of the spin sector on and off plateau manifests in the form of a distinct fermion-fermion interaction between holes in hole-doped antiferromagnets.

In-plateau vs out-of-plateau physics from hole properties.—We consider the signature of the different types of interactions arising from the in-plateau and out-of-plateau states of the spin sector in terms of fermion Green's function renormalization and the spectral function of holes, which is a quantity typically measured by a photoemission experiment when one is interested in the charge degree of freedom. The spectral function, a generalization of the density of states, is defined as $A(\mathbf{k},\omega) = -2\text{sgn}(\omega)\text{Im}G(\mathbf{k},\omega)$, where $G(\mathbf{k},\omega)$ is a renormalized Green's function which embodies the effects of the interaction of fermions with each other and with other degrees of freedom. We will consider an approximation where we geometrically sum a particular family of diagrams involving a series of one-loop fermion self-energy diagrams and obtain the familiar result $G^{-1}(\mathbf{k},\omega) = G_0^{-1}(\mathbf{k},\omega) - \Sigma(\mathbf{k},\omega)$ where in this case $\Sigma(\mathbf{k},\omega)$ is the one-loop self-energy correction to the free fermion Green's function $G_0^{-1}(\mathbf{k},\omega) = \omega - \epsilon_{\mathbf{k}} + i\eta\text{sgn}(|\mathbf{k}| - k_F)$ with η an infinitesimally small positive number to be taken to zero at the end of the calculation [23]. The distinction in the profile of the hole spectral function is what we expect to be a prospective experimental signature that distinguishes the physics of antiferromagnets between within and outside of the plateau.

For the in-plateau case, where we have a local interaction, we compute the one-loop fermion self-energy diagram shown in Fig. 2 with the 4-fermion vertex given in Eq. (11) from which we obtain for the one-loop self-energy $\Sigma(\mathbf{k},\omega) = \int[d^3q/(2\pi)^3]G_0(q)V(k,q)$ where we have to take into account the fact that there are four equivalent configurations of the Feynman diagram in Fig. 2, contributing to $\Sigma(\mathbf{k},\omega)$. The resulting spectral function is demonstrated in Fig. 4(a). We observe that with the local (or short-range) interaction of the in-plateau state, the sharp spectral peak of free fermions is not significantly broadened or dispersed.

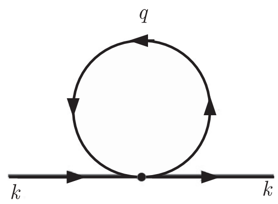

FIG. 2. One-loop self-energy diagram in the in-plateau case with its local fermion-fermion interaction.

For the out-of-plateau case, the one-loop self-energy diagrams are shown in Fig. 3 [23] where the nonlocal long-range interaction is represented by a wavy line. The kernel is given by Eq. (10) with $q = k = k'$ as the momentum frequency of the spin sector's gauge field which mediates the long-range interaction; k''', k''''' are the momenta frequencies of the scattered fermions. From this expression, it is clear that the contribution of the tadpole diagram in Fig. 3(a) vanishes because momentum conservation forces $q = 0$. The expression for the nonvanishing diagram in Fig. 3(b) is $\Sigma(k) = \int[d^3q/(2\pi)^3]G_0(k-q)V(k,q)$ with $V(q,k)$ given in Eq. (10) and where we should note that there are two equivalent configurations of this diagram with equal contribution. The self-energy is both momentum and frequency dependent, reflecting the noninstantaneousness of the algebraic long-range interaction.

We show the resulting profile of $A(\omega)$ at a fixed $\mathbf{k}$ in Fig. 4(b) for this off-plateau case with quadratic hole dispersion. We notice that, due to the algebraically decaying long-range fermion-fermion interaction, the spectral weight is heavily broadened compared to that of free noninteracting fermions which has a hallmark delta function peak. The spectral peak broadening increases with the strength of the coupling to the gauge field represented by gauge charge e_g and also the Goldstone mode's total energy bandwidth $\delta q_0 \sim 2v_b\Lambda$, where 2Λ is the total momentum bandwidth. In the original microscopic spin model Eq. (3), this is achieved for large $J, D \gg h$. Comparing the two cases, it can be seen that the hole spectral function in the out-of-plateau state is much more significantly broadened and suppressed compared to that of the in-plateau state. This broadening reflects the effects of Goldstone bosons which survive outside the plateau and mediate the long-range interaction. We then consider the more realistic finite

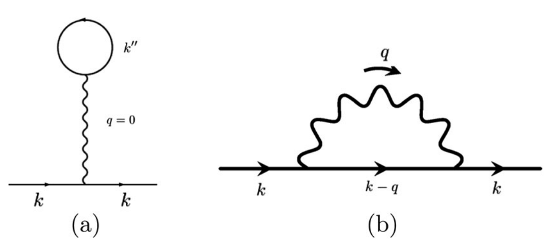

FIG. 3. One-loop self-energy diagrams in the out-of-plateau case where the fermion interaction is long ranged. (a) The tadpole diagram. (b) The bubble diagram.

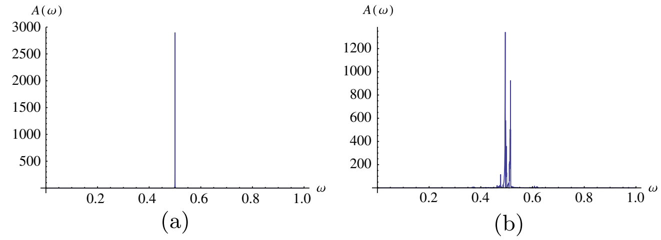

FIG. 4 (color online). Spectral function $A(\omega)$ at a fixed $|\mathbf{k}|$ for quadratic dispersion around Fermi point (a) in the in-plateau case and (b) in the out-of-plateau case [24].

hole-doping situation with its linear dispersion with results shown in Figs. 5(a) and 5(b) giving the same conclusions.

Discussion.—We have demonstrated that the fermion spectral function of hole-doped antiferromagnets can be used as a direct probe of on-plateau vs off-plateau physics of the spin sector. We have shown that within the plateau the spin sector generates a local fermion-fermion interaction while outside the plateau it generates a long-range fermion-fermion interaction with both density-density and dipolar contents. This difference manifests in the spectral function of the holes. In particular, our result predicts that the hole spectral function for the in-plateau case remains a sharp delta function hallmark of the free fermion spectral function with negligible broadening, whereas outside the plateau, the hole spectral function is significantly broadened and reduced in height, subject to an appropriate sum rule. We also predict that finite hole doping will shift the magnitude of plateaus.

With the presence of long-range algebraic interactions, there is a possibility for the formation of Wigner crystals [25] of holes, when the density-density interaction, which is indeed repulsive in this case, dominates over the dipolar interaction and kinetic energies. In contrast to the usual Coulomb case, however, based on dimensional analysis, we expect the Wigner crystal to occur at a high density of holes rather than a low density. This is due to the fact that the algebraic interaction decays as $V(r) \sim 1/r^3$ rather than the usual $V(r) \sim 1/r$, while kinetic energy goes as $1/r^2$.

Compared with the 1D case, it is expected that, other than the clear differences in technical details, the distinction in the behavior of the spectral function on and off plateaus will be less discernible, due to the Luttinger (non-Fermi) liquid

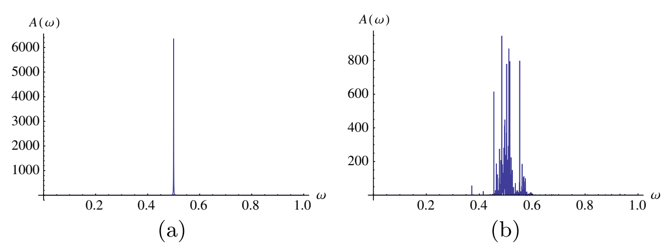

FIG. 5 (color online). Spectral function $A(\omega)$ at a fixed $|\mathbf{k}|$ for linearized dispersion at finite doping (a) in the in-plateau case and (b) in the out-of-plateau case [24].

behavior. Our results qualitatively agree with hole spectral function theoretical calculations for antiferromagnets in underdoped cuprates (at zero field) treated with a slave-particle approach, where similar broadening arises due to the nonlocal (despite finite-ranged few nearest-neighbor) interactions [26], and are confirmed experimentally [27]. As photoemission studies on hole-doped antiferromagnets with plateaus at a finite field themselves have not yet been available, we would like to propose candidate materials: 2D antiferromagnet compounds $SrCu_2(BO_3)_2$ [28] and $(CuBr)Sr_2Nb_3O_{10}$ [29], which are very promising compounds for testing our theoretical predictions as they are 2D antiferromagnetic materials that have been shown to display plateaus.

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[15] Starting from a spin model with easy plane anisotropy under a magnetic field [4] as given in Eq. (3), it can be shown that for 2D antiferromagnets on a square lattice with lattice spacing a,

$$K_\tau = \frac{1}{2a^2(4J+D)}, \qquad K_r = J(S^2 - m^2). \tag{14}$$

[16] In the rest of this paper, $k's$ represents the set of all momenta frequencies appearing in the expression: $k's = k, k', k'', \ldots$, $\int_{k's} = \int d^3k/(2\pi)^3 \int d^3k/(2\pi)^3 \int d^3k/(2\pi)^3 \ldots$ where $d^3k = dk_0 d^2\mathbf{k}$, and $\delta(\sum_{k's}) = \delta(k - k' + k'' \ldots)$ imposing the conservation of momentum frequency.
[17] In this case, the gauge coupling $e_{gx} = e_{gy} \sim S(S-m)/m$, while $e_{g\tau} \sim g_2$ where

$$g_2 = \left[\frac{1}{2S}\left(\frac{S-m}{a^2}\right) + \frac{2tSm^{2S-1}\cos k_F a}{(1-\frac{\delta}{2S})(4J+D)}\right] \tag{15}$$

at doping level δ. Lorentz invariant theory requires $e_{g\tau} = e_{gx} = e_{gy} = e_g$ which can be achieved by appropriate rescaling of space-time.
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[20] In this work, we define Coulomb interaction to be that derived from Gauss law $\nabla.\mathbf{E} = -\nabla^2 V = \rho/\epsilon_0$, giving, for particles of charge e,

$$H = \int_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}} \bar{\psi}_{\mathbf{k}_2-\mathbf{q}} \psi_{\mathbf{k}_2} \frac{4\pi e^2}{q^2} \bar{\psi}_{\mathbf{k}_1+\mathbf{q}} \psi_{\mathbf{k}_1}.$$

The (true) long-range nature is signaled by the divergence of the kernel $V(q) = (4\pi e^2/q^2) \to \infty$ as $q \to 0$. Weaker divergence, e.g., $V(q) \to V(0)$ with $0 < V(0) < \infty$ as $q \to 0$, indicates a faster-decaying long-range interaction.
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