Neutron scattering in the hole-doped cuprate superconductors

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The occurrence of a neutron resonance energy is a common feature of unconventional superconductors. In turn, the low-temperature incommensurate sharp peaks observed in the inelastic neutron scattering of La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) correspond to four rods symmetrically distributed around $[\pi, \pi]$. Here it is shown that within the virtual-electron pair quantum liquid recently introduced the neutron resonance energy and the LSCO low-temperature incommensurate sharp peaks are generated by simple and closely related spinon processes. Our results indicate that in LSCO the neutron resonance energy either does not occur or corresponds to a lower energy $\approx 17$ meV.

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Evidence is provided in Ref. [1] that the occurrence of a neutron resonance energy in different classes of unconventional superconductors follows from superconductivity being mediated by magnetic fluctuations. The spin-wave spectrum of the parent compound La$_2$CuO$_4$ (LCO) is quantitatively described by the square-lattice quantum liquid (SLQL) of Ref. [2]. Such a liquid refers to the Hubbard model on the square lattice with effective transfer integral $t$ and on-site repulsion $U$, defined in a subspace that contains its one- and two-electron excitations. Within the SLQL the spinon spectrum that generate the spin-wave spectrum are very simple, yet they lead to the same spectrum as Ref. [4], where it is derived by summation of an infinite set of ladder diagrams. The virtual-electron pair quantum liquid (VEPQL) recently introduced in Ref. [5] refers to the SLQL perturbed by small three-dimensional uniaxial anisotropy. Within it, a long-range superconducting order emerges, mediated by magnetic fluctuations. The description of both the SLQL and VEPQL in terms of charge $c$ fermions, spin-singlet two-spinon $s$ fermions, and independent spinons [3] profits from the extended global $SO(3) \times SO(3) \times U(1) = [SO(4) \times U(1)]/\mathbb{Z}_2$ symmetry found recently in Ref. [6] for the Hubbard model on any bipartite lattice. The new found $U(1)$ symmetry is that broken at the critical temperature $T_c$. In Refs. [3, 5] the VEPQL is shown to successfully describe the universal unusual properties of the hole doped cuprates, including the normal-state linear-$T$ resistivity [7].

In this Letter strong evidence is provided that combination of the simple $s$ fermion processes studied in Ref. [5] for hole concentration $x = 0$ with the contraction and deformation of the $s$ boundary line upon increasing $x$ leads for approximately $x \in (x_c, x_{c1})$ to sharp peaks in the spin-triplet spectral weight distribution. They correspond to four rods symmetrical distributed about $\bar{\pi} = [\pi, \pi]$, alike those observed in the inelastic neutron scattering of La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) [8, 9]. Here $x_c \approx 0.05$ and $x_{c1} \approx 1/8 = 0.125$. Importantly, a second type of closely related processes whose spectrum we evaluate for approximately $x \in (x_c, x_{c2})$ where $x_{c2} \approx 0.16$ leads to a sharp spectral feature centered at $\bar{\pi}$. Within the VEPQL scheme it is identified with the neutron resonance energy observed in the four representative systems other than LSCO considered in the studies of Ref. [3]: YBa$_2$Cu$_2$O$_{6+\delta}$ (YBCO 123), Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (Bi 2212), HgBa$_2$CuO$_{4+\delta}$ (Hg 1201), and Tl$_2$Ba$_2$CuO$_{6+\delta}$ (Tl 2201). (Due to disorder effects [10], for $x < x_c$ the momentum-space position of the peaks predicted here for LSCO is rotated by an angle $\pi/4$.)

For the $x = 0$ and spin-density $m = 0$ absolute ground state the $s$ band coincides with an antiferromagnetic reduced Brillouin zone such that $|q_x| + |q_y| \leq \pi$. Its $s$ boundary-line momenta $q_{s1}$ have Cartesian components obeying the equations $q_{s1x} \pm q_{s1y} = \pm, \mp \pi$. In turn, the following equations derived in Ref. [5] for small values of $x$ and $U/4t \geq u_0$, which due to the $s$ boundary line contraction upon increasing $x$ are obeyed by the Cartesian components of the momenta belonging to that line and pointing in and near the nodal directions, remain a good approximation for $x \in (x_c, x_{c1})$.

$$q_{s1x1} \pm q_{s1x2} = \pm, \mp(1 - x)\pi, \quad U/4t \geq u_0 \approx 1.302.$$  \hfill (1)

(Unlike for one-electron excitations, for the spin excitations considered here the $s$ band momenta are independent of the doublidity $d = \pm 1$ [3, 5, 6, 7].) The $s$ band is full for the initial $m = 0$ ground state and displays two holes for the spin excitations. The corresponding VEPQL general spin spectrum derived in Ref. [3] reads,

$$\delta E_{\text{spin}} = -\epsilon_{s1}(\vec{q}') - \epsilon_{s1}(\vec{q}'') - \epsilon_{s1}(\vec{q}'), \quad \delta \vec{F} = [\delta \vec{q}^0 - \vec{q}' - \vec{q}''],$$

$$\delta \vec{q}^0 = \pm \left[ \frac{\pi(1 - x)}{\pm \pi(1 - x)} \right], \quad x = 0, x > x_c.$$  \hfill (2)

In the energy spectrum $\epsilon_{s1}(\vec{q})$ denotes the $s$ fermion energy dispersion [3, 5, 6, 7]. Our results refer to momenta $\vec{q}' \approx \vec{q}_{s1}$ and $\vec{q}'' \approx \vec{q}_{s1}$ at or near the $s$ boundary line for which according to the results of Ref. [3, 5, 6, 7], $\epsilon_{s1}(\vec{q}') - \epsilon_{s1}(\vec{q}'') \approx |\Delta| \cos 2\phi' + \cos 2\phi'' + 2|\Omega| \sin 2\phi$. Here the angles $\phi'$, $\phi''$, and $\phi$ are associated with the directions of $\vec{q}'$, $\vec{q}''$, and $\vec{q} = [1/2](\vec{q}' - \vec{q}'')$, respectively. Moreover, $|\Delta| = g_1 \Delta_0$ and $|\Omega| = \gamma_d g \Delta_0/(1 - |x/x_c|)[4g/\gamma_c]$ are
the spinon and superconducting VEP pairing energy per electron, respectively, [3]. The amplitudes $g_1 = |(e^{i \theta_1})|$ and $g = |(e^{i \theta})| = |(e^{i(\theta_0 + \theta_1)})|$ in such energy expressions are averages over the whole system of phase factors fully controlled by the quantum fluctuations of the VEP phases $\theta_j$ and $\gamma_c = (1 - x_c/x_s)$, and $\gamma_d$ such that coefficient $\gamma_c < \gamma_d < 1$ is a suppression coefficient. The latter coefficient accounts for the effects of intrinsic disorder or superfluid-density anisotropy, which for $x \in (x_c, x_s)$ are small [3]. The parameters appropriate to the representative systems are $U/4t \approx 1.525, t \approx 295$ meV, $x_c \approx 0.05$, and $x_s \approx 0.27$, so that $\Delta_0 \approx 42$ meV for LSCO and $\Delta_0 \approx 84$ meV for the four systems other than LSCO [2]. The VEPQL critical temperature $T_c$ above which there is no long-range superconducting order and the pseudogap temperature $T^*$ above which there is no short-range spin order read $T_c = \gamma_d \Delta_0/2k_B$ and $T^* \leq \gamma_1|\Delta_0/k_B|$, respectively. Here $\gamma = g_{T=0} \approx [(x_s - x_c)/(x_s - x_c)] \gamma_1$ and $\gamma_1 = g_{1,T=0} \approx (1 - x_s/x_s)$ for $x \in (x_c, x_s)$.

Within the present status of both the SLQL and VEPQL schemes one cannot calculate explicitly matrix elements of the two-electron spin-triplet operator $\langle \delta \mathbf{q}, | \mathcal{V}_{\text{SLQL}} \rangle$ or $\langle \delta \mathbf{q}^', \mathcal{V}_{\text{VEPQL}} \rangle$, for the SLQL. At $c$-fermion momentum $x = 0$ and $m = 0$ the $c$-fermion and two-spinon $s_1$ fermion description of Refs. [3, 5] renders a very complex many-electron spin problem into a much simpler one. (Some of our results remain valid for at least $x \in (x_c, x_{op})$.) Indeed, the $c$ and $s_1$ fermion momentum values are close to good quantum numbers for the VEPQL used in our studies [3]. Our results are valid for $U/4t \geq u_0 \approx 1.3$. The lack of long-range antiferromagnetic order in the initial $x \neq 0$ and $m = 0$ ground state [3, 5] implies that now the sharpest spectral features do not refer to coherent spin weight and thus are not $\delta$-function like. Our main conjecture is that for hole concentrations approximately in the range $x \in (x_c, x_{c1})$ such sharpest spin features are generated as well by processes under which: (i) The two $s_1$ fermion holes in the general spin spectrum of Eq. (2) emerge at momenta $\vec{q}'$ and $\vec{q}''$ in the intersection of the lines $[q_{x_1}, \pm \pi/2]$ or $[\pm \pi/2, q_{x_2}]$ with the $s_1$ boundary line. (ii) The momentum part $\vec{q} = [1/2](\vec{q}' - \vec{q}'')$ of such momenta corresponding to the spinon relative motion in the broken pair is a $s_1$ boundary-line nodal momentum. It follows that both the momenta $\vec{q}'$ and $\vec{q}''$ and the corresponding relative momentum $\vec{q} = [1/2](\vec{q}' - \vec{q}'')$ must belong to the $s_1$ boundary line. Both the conditions (i) and (ii) are met at $x = 0$. For $x \in (x_c, x_{c1})$ such a conjecture is confirmed below to lead to results fully consistent with the low-temperature neutron inelastic scattering of the five representative hole-doped cuprate superconductors. The incommensurability effects bring about a finite momentum part $\delta \vec{q} = (\vec{q}' + \vec{q}'')$ referring to the motion of the center of mass of the broken spinon pair.

Following our above discussion, we consider that alike for $x = 0$ and $m = 0$, for $x \in (x_c, x_{c1})$ and $m = 0$ the sharpest spin spectral peaks refer to processes meeting the above conditions (i) and (ii). From use of Eq. (11), one finds that the condition (i) that the momenta $\vec{q}'$ and $\vec{q}''$ are in the intersection of the lines $[q_{x_1}, \pm \pi/2]$ or $[\pm \pi/2, q_{x_2}]$ with the $s_1$ boundary line is met by $s_1$
boundary-line momenta $\mathbf{q}'$ and $\mathbf{q}''$ of the general form,

$$\delta \mathbf{q}_{N,a,l,l'} = l' \left[ \frac{\pi}{2} \right] ; \delta \mathbf{q}_{B_{B_{s}}} = l \left[ \frac{\pi}{2} \right] ,$$

where $l, l' = \pm 1$. Furthermore, the condition (ii) that the corresponding relative momentum $\mathbf{q} = [1/2](\mathbf{q}' - \mathbf{q}'')$ is a $s1$ boundary-line momenta is met by the momentum pairs $\mathbf{q}' = \mathbf{q}_{N,a,l,l'}$ and $\mathbf{q}'' = \mathbf{q}_{N,b,-l',l'}$. Indeed, such momenta can be written as,

$$\delta \mathbf{q}_{N,a,l,l'} = \frac{1}{2} \delta \mathbf{q}_{N,1,1,l,l'} ; \delta \mathbf{q}_{N,b,-l',l'} = -\delta \mathbf{q}_{N,1,1,l,l'} + \frac{1}{2} \delta \mathbf{q}_{N,1,1,l,l'} ,$$

Here the relative momentum,

$$\delta \mathbf{q}_{N} = l \left[ \frac{\pi}{2} \right] ; l, l' = \pm 1 ,$$

is indeed a $s1$ boundary-line momentum pointing in nodal directions. It corresponds to the relative motion of the spinons in the broken pair. In turn, the momentum,

$$\delta \mathbf{q}_{N,1,1,l,l'} = \delta \mathbf{q}_{N,1,1,l,l'} + \frac{1}{2} \delta \mathbf{q}_{N,a,l,l'} + \frac{1}{2} \delta \mathbf{q}_{N,b,-l',l'} ,$$

corresponds to the motion of the center of mass of such a pair. The momentum $\delta \mathbf{q}_{N,1,1,l,l'}$ vanishes at $x = 0$, consistently with vanishing for the processes leading to the $x = 0$ sharpest spin spectral features.

There are two types of closely related $s1$ fermion processes for which $\mathbf{q}' = \mathbf{q}_{N,a,l,l'}$ and $\mathbf{q}'' = \mathbf{q}_{N,b,-l',l'}$ in the general spin spectrum [2]. For the first process type $\delta \mathbf{q}_{0} = \pm (1-x)[\pi, \pi]$ in that spin spectrum. We straightforwardly find the following value for the momentum $\delta \mathbf{P}$ of Eq. [2] for hole concentrations approximately in the range $x \in (x_{c}, x_{c1})$,

$$\delta \mathbf{P} = \delta \mathbf{P}_{c} - \delta \mathbf{q}_{N,a,l,l'} - \delta \mathbf{q}_{N,b,-l',l'} = \delta \mathbf{P}_{c} - \delta \mathbf{q}_{N,1,1,l,l'} ,$$

$$= \pm \frac{\pi (1-x)}{\pi (1-x)} - \frac{1}{1} \pm \frac{1}{1} .$$

Owing to the lattice discrete translational symmetry, corresponding processes originated by adding to those a suitable reciprocal-lattice vector $\mathbf{G} = [2\pi, 2\pi]$ give rise to the excitation momenta,

$$\delta \mathbf{P} = \pm \frac{\pi (1-x)}{\pi (1-x)} - \frac{1}{1} \pm \frac{2\pi}{2\pi} .$$

As discussed below, this first type of processes correspond to momentum locations identical to those of the sharp low-temperature incommensurate peaks in the inelastic neutron scattering of LSCO.

The corresponding incommensurability is defined as $\delta_{inc} = \frac{1}{2\pi} |\delta \mathbf{P} - \delta \mathbf{P}^{*}|$. Here $\delta \mathbf{P}$ stands for any of the excitation momenta of Eqs. [7] and [8]. We now use the $s1$ boundary line nodal momentum $\mathbf{q}_{N,a}$ expression provided in Ref. [3] to derive the following corresponding expression of the incommensurability valid for the extended hole concentration range $x \in (x_{c}, x_{c1})$,

$$\delta_{inc} = \frac{1}{2\pi} |\mathbf{P} - \delta \mathbf{P}^{*}| ,$$

Hence, for the present hole concentration range $x \in (x_{c}, x_{c1})$ and for instance for the quadrant for which the components the momenta $\delta \mathbf{P}$ are such that $\delta \mathbf{P}_{x_{c}} , \delta \mathbf{P}_{x_{c1}} \geq 0$, the sharpest peaks of the spin spectral weight distribution correspond within our above generalization of the $x = 0$ processes found in Ref. [3] to four 2D rods at $\delta \mathbf{P} = [\pi \pm 2\pi \delta_{inc}, \pi]$ and $\delta \mathbf{P} = [\pi, \pi \pm 2\pi \delta_{inc}]$. Those are symmetrical distributed about $\pi = [\pi, \pi]$.

A second type of closely related processes that also obey the above conditions (i) and (ii) refer to the choices $\delta \mathbf{q}_{0} = \pm (1-x)[\pi, -\pi]$ in the general spin spectrum [2] for $l, l' = \mp 1$,

$$\delta \mathbf{P} = \pm \frac{\pi (1-x)}{\pi (1-x)} - \frac{1}{1} \pm \frac{\pi}{\pi} .$$

This spectrum is expected to remain a good approximation at least for $x \in (x_{c}, x_{op})$.

The energy spectra corresponding to the momentum spectra of Eqs. [7] and [8] and spectrum of Eq. [10] have the same form. From the use of the general spin spectrum of Eq. [2] one finds for zero temperature,

$$\delta E_{spin} = -\epsilon_{s1}(\mathbf{q}_{N,a,l,l'}) - \epsilon_{s1}(\mathbf{q}_{N,b,-l',l'}) \approx |\Delta| \cos 2\phi' + \cos 2\phi'' + 2|\Omega| \sin 2\phi = 2|\Omega| .$$

Here the angles $\phi'$ and $\phi''$ and the angle $\phi$ are associated with the directions pointed by the momenta $\mathbf{q}' = \mathbf{q}_{N,a,l,l'}$ and $\mathbf{q}'' = \mathbf{q}_{N,b,-l',l'}$ of Eq. [1] and the relative momentum $\delta \mathbf{q} = \delta \mathbf{q}_{N,a}$ of Eq. [5], respectively. The surprisingly simple energy spectrum $\delta E_{spin} \approx 2|\Omega|$ associated with both the excitation momenta of Eqs. [7] and [8] and Eq. [10] follows from $\cos 2\phi' = -\cos 2\phi''$ and $|\sin 2\phi| = 1$ for the $s1$ band momenta under consideration. Within the VEPQL scheme the second type of processes whose spectrum is given in Eqs. [10] and [11] generate the neutron resonance energy observed in YBCO 123, Bi 2212, Hg 1201, and Tl 2201, as discussed below.

For temperatures below $T_{c}$ and a well-defined temperature-dependent range the spectrum [11] has the
same form except that the amplitude \( g \) and thus the pairing energy \( 2|\Omega| \) decrease upon increasing \( T \) and vanish for temperatures above \( T_c \). Hence for temperatures in the range \( T \in (T_c, T^*) \) below the pseudogap temperature \( T^* \) the spin energy \( \delta E_{\text{spin}} \) vanishes, \( \delta E_{\text{spin}} \approx 0 \).

The low-temperature incommensurate peaks in the inelastic neutron scattering of LSCO are for \( x \in (x_c, x_{c1}) \approx (0.05, 0.125) \) observed precisely at the momentum values \( \delta \vec{P} = [\pi \pm 2\pi \delta \vec{P}_{nc}], \pi \) and \( \delta \vec{P} = [\pi, \pi \pm 2\pi \delta \vec{P}_{nc}] \) \([8, 9]\) of Eqs. (7) and (8). The LSCO experimental dependence of \( \delta \vec{P}_{nc} \) on \( x \) is studied in Refs. \([8, 9]\). For instance the Sr-doping experimental points of Fig. 37 (a) of Ref. \([8]\) confirm that for LSCO the theoretical magnitudes \( \delta \vec{P}_{nc} \approx x \) for \( x \in (x_c, x_{c1}) \approx (0.05, 0.125) \) and \( \delta \vec{P}_{nc} \approx x_{c1} = 1/8 \approx 0.125 \) for \( x \in (x_{c1}, x_s) \approx (0.125, 0.27) \) given in Eq. (9) are indeed approximately valid.

At zero temperature the excitation energy corresponding to the excitation momenta \( \delta \vec{P} \) of Eqs. (7) and (8) reads \( \delta E_{\text{spin}} \approx 2|\Omega| \), as given in Eq. (11). Upon increasing the temperature \( T \) the phase-coherent virtual-electron pairing energy \( 2|\Omega| \) decreases and vanishes as \( T \to T_c \). Therefore, for \( x \in (x_c, x_{c1}) \) and for the low-energy \( \delta E_{\text{spin}} \approx 0 \) regime associated with the spectrum \( \delta \vec{P}_{nc} \) for temperatures \( T \geq T_c \) at which \( 2|\Omega| = 0 \) the intensity of the incommensurate peaks as a function of \( T \) has a sharp maximum at \( T \approx T_c \). It diminishes rapidly toward zero as \( T \) is lowered, consistently with the opening of the spin-spectrum nodal gap associated with the phase-coherent virtual-electron pairing energy \( 2|\Omega| \). It refers to the spectrum \( \delta E_{\text{spin}} \approx 2|\Omega| \) of Eq. (11). This is again the behavior observed in LSCO \([8]\).

In YBCO 123 the width of the scattering makes it difficult to observe any incommensurability. In that material and also in Bi 2212, Hg 1201, and Tl 2201 a single sharp spin spectral feature centered at \( \vec{\pi} = [\pi, \pi] \) is observed. Within the VEPQL it refers to the spectrum given in Eqs. (10) and (11) generated by the above second type of excitations. Their excitation energy is at low temperature given by \( \delta E_{\text{spin}} \approx 2|\Omega| \approx 2|\Omega| \big|_{T=0} \). Its maximum magnitude \( \delta E_{\text{spin}} \approx 2|\Omega|^{\text{max}} \approx 2|\Omega|^{\text{max}} \big|_{T=0} \) occurs at the optimal hole concentration \( x_{op} = 0.16 \). The theoretical energy \( 2|\Omega|^{\text{max}} \approx \gamma_{\min}^2 T_c \Delta_0 / 2 \approx 5k_B T_c^{\text{max}} \) calculated for the parameters appropriate to YBCO 123, Bi 2212, Hg 1201, and Tl 2201 reads \( 2|\Omega|^{\text{max}} \approx 40 \) meV for all of them. This agrees quantitatively with the neutron resonance energy \( 2|\Omega|^{\text{max}} \) observed in such materials, which is given by \( 39 - 41 \) meV \([11]\).

We emphasize that the two types of closely related processes considered here only differ in the sign \( \pm \) of the factor \( [\pi, \mp \pi] \) appearing in the momentum \( \delta \vec{Q}_{nc} = \pm (1 - x)[\pi, \pm \pi] \) of the general spin spectrum \([2]\). The first type of excitation is difficult to observe in the four systems other than LSCO due to the scattering width. The neutron resonance energy was not observed in LSCO. If the second type of excitations with spectrum given in Eqs. (10) and (11) occurred in LSCO the theoretical energy calculated for the parameters appropriate to it would be \( 2|\Omega|^{\text{max}} \approx 17 \) meV. One possibility is that due to matrix-elements issues specific to the LSCO physics only the excitations with spectrum given in Eqs. (10), (11), and (11) generate sharp spin spectral features. Whether a smaller neutron resonance energy \( 2|\Omega|^{\text{max}} \approx 17 \) meV occurs in LSCO is a problem that deserves further experimental investigations.

Hence we conclude that within the conjecture that the sharpest spin spectral features are generated for \( x \in (x_c, x_{c1}) \) by a type of two-spinon s1 fermion processes similar to those found in Ref. \([8]\) for \( x = 0 \) and \( m = 0 \), the VEPQL scheme of Refs. \([8, 9]\) leads to remarkable quantitative agreement with the low-temperature incommensurate peaks in the inelastic neutron scattering of LSCO \([8]\). Excellent quantitative agreement between our theoretical predictions and the neutron resonance energy observed in YBCO 123, Bi 2212, Hg 1201, and Tl 2201 is also achieved. Importantly, our results reveal that the low-T incommensurate sharp peaks and the neutron resonance energy observed in LSCO and the remaining four representative systems, respectively, are generated by closely related processes. They are two faces of the same phenomenon. Our results strongly suggest that the \( c \) and s1 fermion description used in the studies of this Letter renders a very complex spin-spectrum many-electron problem into a much simpler problem in terms of suitable two-s1-fermion-hole s1 band processes. This is consistent with the VEPQL momentum values of the \( c \) and s1 fermions being close to good quantum numbers \([8, 9]\).

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