

Pinning of dynamic spin density wave fluctuations in the cuprate superconductors

Anatoli Polkovnikov,¹ Matthias Vojta,² and Subir Sachdev¹

¹*Department of Physics, Yale University, P.O. Box 208120, New Haven CT 06520-8120*

²*Theoretische Physik III, Elektronische Korrelationen und Magnetismus, Universität Augsburg, 86135 Augsburg, Germany*

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We present a theory of the pinning of dynamic spin density wave (SDW) fluctuations in a d -wave superconductor by local imperfections which preserve spin-rotation invariance, such as impurities or vortex cores. The pinning leads to static spatial modulations in spin-singlet observables, while the SDW correlations remain dynamic: these are the ‘Friedel oscillations’ of a spin-gap antiferromagnet. We connect the spectrum of these modulations as observed by scanning tunnelling microscopy to the dynamic spin structure factor measured by inelastic neutron scattering.

Many studies of the cuprates assume that high temperature superconductivity is best understood by a theory of doping mobile charge carriers into a Mott insulator which is paramagnetic [1] *i.e.* a Mott insulator with no static spin moment on any site and dynamic antiferromagnetic spin density wave (SDW) correlations. Studies of paramagnetic Mott insulators on the square lattice of Cu ions [2] showed that the most promising candidates have broken translational symmetry (and confinement of $S = 1/2$ spinon excitations) associated with the appearance of spontaneous bond charge order. Here, and henceforth, we define the term “charge order” very generally: there is a periodic spatial modulation in observables which are invariant under spin rotations and time reversal, such as local electron/hole density of states (LDOS), the spin exchange energy, the pairing amplitude, or the electron kinetic energy contained in a link of the square lattice; the modulation in the total charge density may well be unobservably small because of screening by the long-range Coulomb interactions.

Ref 2 studied the doping of the charge-ordered paramagnetic Mott insulator: superconductivity co-existed with charge order for a finite range of carrier concentrations (δ), and a d -wave superconductor with the full square lattice symmetry appeared above a critical δ . This, and other theoretical and experimental studies have concluded that the low temperature properties of this d -wave superconductor at optimal δ are qualitatively identical to those of a BCS superconductor obtained by the Cooper instability of a metallic Fermi liquid. This conclusion raises the question of whether the connection to the Mott insulator is even necessary in a description of the low temperature properties of the superconductor at or above optimal δ .

A number of works [3] argued that memory of the Mott insulator should survive in and around vortices in superconducting order: the suppression of superconductivity in the vortex core implies that the Cooper pairs are not condensed, but the electrons should still strive to retain the exchange correlation energy of the Mott insulator.

This reasoning, and the studies of the doped paramagnetic Mott insulator [2], led to the suggestion [4] that the static charge order, along with dynamic SDW correlations, should appear near vortex cores.

Hoffman *et al.* [5] introduced a novel scanning tunnelling microscopy (STM) technology of atomically registered spectroscopic mapping. Applied to slightly overdoped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$, they detected LDOS modulations around the vortex cores at wavevectors $\mathbf{K}_{cx} = (\pi/2, 0)$ and $\mathbf{K}_{cy} = (0, \pi/2)$ (the square lattice spacing has unit length and this modulation has a period of four lattice spacings), co-existing with well established superconductivity [6]. Bulk charge order with this, and related, periods has been discussed in insulating/superconducting paired hole states from a number of different theoretical perspectives [2, 4, 7–12]. Neutron scattering studies of the optimally doped cuprates have not (so far) seen dynamic or static charge order, but do see collinear SDW fluctuations at wavevectors $\mathbf{K}_{sx} = (3\pi/4, \pi)$ and $\mathbf{K}_{sy} = (\pi, 3\pi/4)$ and at energies above a spin gap Δ . On symmetry grounds [13], collinear SDW correlations are accompanied by charge order correlations at wavevectors $2\mathbf{K}_{sx,y}$, which equal the values of $\pm\mathbf{K}_{cx,y}$, modulo reciprocal lattice vectors. This connection was used [14] to describe the spatial envelope of the charge order in the doped Mott paramagnet by the pinning of a ‘sliding’ degree of freedom of the SDW (the spin-rotation degree of freedom is not pinned and remains dynamic) by imperfections, such as vortex cores.

This paper presents a description of the energy dependence of the LDOS measured in STM in a simple Gaussian model of the pinning of dynamic SDW fluctuations. We connect the spectroscopic information contained in the STM observation at wavevectors $\mathbf{K}_{cx,y}$ to the inelastic neutron scattering spectra at wavevectors $\mathbf{K}_{sx,y}$. Our theory applies to pinning by impurities and most other imperfections that preserve spin rotation invariance. It also applies to pinning by vortex cores, but neglects the Doppler shift in the quasiparticle energies induced by the superflow [15]: this shift will produce spatial modulations

in the LDOS only on the scale of the superflow variations, and not at the wavevectors $\mathbf{K}_{cx,y}$, and so its neglect is justifiable. Our results should be distinguished from other recent proposals [16] which assume *static* SDW order, for which there is no direct evidence in the system of Ref. 5.

We begin by identifying the complex order parameters, $\Phi_{x\alpha}$, $\Phi_{y\alpha}$ ($\alpha = x, y, z$ extends over the directions in spin space) for SDW fluctuations; the spin operator on the lattice site \mathbf{r} is

$$S_\alpha(\mathbf{r}, \tau) = \text{Re} \left[e^{i\mathbf{K}_{sx} \cdot \mathbf{r}} \Phi_{x\alpha}(\mathbf{r}, \tau) + e^{i\mathbf{K}_{sy} \cdot \mathbf{r}} \Phi_{y\alpha}(\mathbf{r}, \tau) \right],$$

where τ is imaginary time. We use a Gaussian action for $\Phi_{x,y\alpha}$ fluctuations:

$$\mathcal{S}_\Phi = T \sum_{\mathbf{q}, \omega_n, \alpha} \chi_x^{-1}(\mathbf{q}, \omega_n) |\Phi_{x\alpha}(\mathbf{q}, \omega_n)|^2 + (x \rightarrow y); \quad (1)$$

we have Fourier transformed from (\mathbf{r}, τ) to wavevectors \mathbf{q} and Matsubara frequencies ω_n at a temperature T . The dynamic spin susceptibilities $\chi_{x,y}$ will be inputs from which we will deduce the dynamic structure of the pinned charge order. However, this should not be interpreted as a causal connection from the SDW fluctuations to the charge order; rather, our method relies on the assumed proximity of the superconductor to a quantum transition to a superconducting state with long-range SDW order [2, 6]. The presence of such a quantum critical point, and the values of $\mathbf{K}_{sx,y}$ near it, are determined by a complicated interplay between spin and charge correlations in the superconductor and the proximate Mott insulator. A corresponding theory using the charge density wave order parameter can also be developed near a charge-ordering transition in the superconductor; this is not discussed here and it yields results related to those in [14]. We will take a simple functional form for $\chi_{x,y}$ (see below), with a spectral weight which vanishes below a spin gap energy Δ (a more accurate form can, in principle, be extracted from neutron scattering experiments). Ref. 6 argued that the value of Δ can be tuned by an applied magnetic field perpendicular to the square lattice layers, and its primary effect is a reduction in Δ .

Invariance under translation by n_x lattice spacings in the x direction (for arbitrary integer n_x) leads to the symmetry $\Phi_{x,\alpha} \rightarrow e^{in_x \pi/4} \Phi_{x,\alpha}$ obeyed by \mathcal{S}_Φ (and similarly for $\Phi_{y\alpha}$). As long as this symmetry is preserved, no observable will exhibit static charge order at wavevectors $\mathbf{K}_{cx,y}$. However, this sliding translation symmetry is broken by any imperfection (vortex core or impurity) that may be centered near $\mathbf{r} = \mathbf{r}_0$, provided the spatial extent of the imperfection is not much larger than the charge order period (4 lattice spacings). We account for such an imperfection by adding a pinning term to the action

$$\mathcal{S}_{\text{pin}} = - \sum_{\alpha} \int d\tau \left[\zeta_x \Phi_{x\alpha}^2(\mathbf{r}_0, \tau) + (x \rightarrow y) + c.c. \right], \quad (2)$$

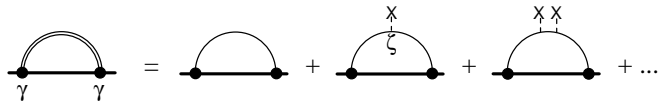


FIG. 1: One-loop diagrams for the self energy of the host conduction electrons. Thick lines are bare conduction electron propagators, a single/double thin line denotes a bare/full SDW propagator, and the cross represents the scattering of the SDW fluctuations by the imperfection pinning term.

where $\zeta_{x,y}$ are complex coupling constants representing the pinning potential. Note that \mathcal{S}_{pin} contains the simplest terms which break the $\Phi_{x,\alpha} \rightarrow e^{in_x \pi/4} \Phi_{x,\alpha}$ symmetry, but preserve spin rotation invariance. Additional terms like $\Phi_{x\alpha}(\mathbf{r}_0, \tau) \Phi_{y\alpha}(\mathbf{r}_0, \tau)$ are also permitted but we will not include them for simplicity; such terms lead to a 90° turn in an SDW fluctuation and can be expected to have a small amplitude on physical grounds—their presence will lead to additional charge order at $\pm \mathbf{K}_{sx} \pm \mathbf{K}_{sy}$. We also note that the theory for the superconductor proximate to a charge ordering transition has a pinning term linear in the charge order parameter.

STM involves tunneling of single electrons, and so to compute the STM spectra we couple the Gaussian SDW fluctuations described by $\mathcal{S}_\Phi + \mathcal{S}_{\text{pin}}$ to the electrons, which we describe by a standard d -wave BCS model:

$$H_{\text{BCS}} = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger [(\varepsilon_{\mathbf{k}} - \mu)\tau^z + \Delta_{\mathbf{k}}\tau^x] \Psi_{\mathbf{k}}. \quad (3)$$

Here $\Psi_{\mathbf{k}} = (c_{\mathbf{k}\uparrow}, c_{-\mathbf{k}\downarrow}^\dagger)$ is a Nambu spinor at momentum $\mathbf{k} = (k_x, k_y)$, $\tau^{x,y,z}$ are Pauli matrices in particle-hole space, and μ is a chemical potential. For the kinetic energy, $\varepsilon_{\mathbf{k}}$ we have first (t) and second (t') neighbor hopping, while we assume a d -wave form for the BCS pairing function $\Delta_{\mathbf{k}} = (\Delta_0/2)(\cos k_x - \cos k_y)$. The full Hamiltonian for the conduction electrons reads

$$H = H_{\text{BCS}} + \gamma \sum_{\mathbf{r}} c_{\mu}^\dagger(\mathbf{r}) \sigma_{\mu\nu}^\alpha c_{\nu}(\mathbf{r}) \times (\Phi_{x\alpha}(\mathbf{r}) e^{i\mathbf{K}_x \cdot \mathbf{r}} + \Phi_{x\alpha}^*(\mathbf{r}) e^{-i\mathbf{K}_x \cdot \mathbf{r}} + (x \rightarrow y)), \quad (4)$$

where σ^α are the Pauli spin matrices, and γ describes the scattering of the Bogoliubov quasiparticles of the superconductor off the SDW fluctuations.

We computed the influence of the collective SDW modes on the single particle properties in the one-loop approximation sketched in Fig 1 with processes of second order in the electron-SDW coupling γ . Because of the breaking of translational symmetry in \mathcal{S}_{pin} , the computations were numerically involved: we used lattices of sizes up to 32×32 with periodic boundary conditions, and numerically inverted matrices in real space to transform the self energy and the Green's function.

Our main results are apparent by considering the linear effect of the lowest order diagram which breaks translational invariance: this is the second diagram on the

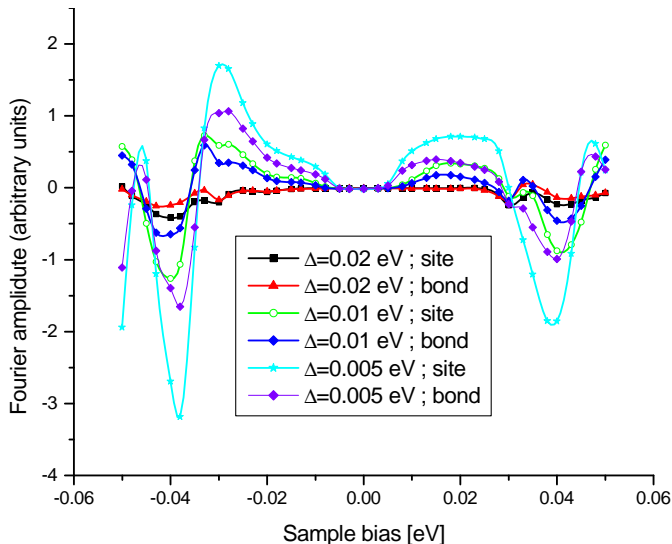


FIG. 2: The $\zeta_{x,y}\gamma^2$ term of (5), as a function of the energy, ω , of the electron. The BCS superconductor is parameterized by hopping strengths $t = -0.15$ eV, $t' = -t/4$, chemical potential $\mu = -0.135$ eV which gives a doping level of about 15%, and a size of the d -wave gap of $\Delta_0 = 40$ meV. Results are shown for different values of Δ , with $c = 0.2$ eV and \mathbf{r}_0 on a square lattice site or bond (results for \mathbf{r}_0 on a plaquette are similar to those on a bond).

r.h.s. of Fig. 1, and is of order $\zeta_{x,y}\gamma^2$. We computed its influence on the LDOS in a theory with $J\chi_{x,y}^{-1} = \omega_n^2 + c^2\mathbf{q}^2 + \Delta^2$ (J is a characteristic spin fluctuation energy scale, and c is a spin-wave velocity) so that, after a Fourier transform to real space, the $\Phi_{x,y}$ propagators became Bessel functions of \mathbf{r} . Following the method of Hoffman *et al.* [5], we computed the energy (ω) dependence of

$$\sum_{\mathbf{r}} e^{-i\mathbf{K}_{cx,y}\cdot\mathbf{r}} \text{Im} c_{\mu}(\mathbf{r}, \omega_n) c_{\mu}^{\dagger}(\mathbf{r}, \omega_n) \Big|_{i\omega_n \rightarrow \omega + i0^+}, \quad (5)$$

the coefficients of the spatial Fourier transform of the LDOS at wavevectors $\mathbf{K}_{cx,y}$. The $\zeta_{x,y}\gamma^2$ term in (5) was evaluated by summations over \mathbf{r} and frequency space. Its values are shown in Fig 2 for a fermion band corresponding to an optimally doped cuprate. This method has the advantage that the values of γ , and $\zeta_{x,y}$ only modify an overall pre-factor of the modulation, and so do not effect the energy dependence of the results in Fig 2. The change in sign of the LDOS at $|\omega| < \Delta_0$ arises from interference between the real and imaginary parts of the bare propagator and the self energy.

We also performed computations in a *different* model in which all the diagrams in Fig 1 were summed. We introduced two *real* three-component fields $\varphi_{x,y\alpha}(\mathbf{r}, \tau) = \text{Re}[e^{i\mathbf{K}_{sx,y}\cdot\mathbf{r}}\Phi_{x,y\alpha}(\mathbf{r}, \tau)]$, with their momenta, \mathbf{k} , extending over the whole Brillouin zone of the square lattice – this simplifies the exact treatment of the pinning term with a T matrix. The bulk fluctuations

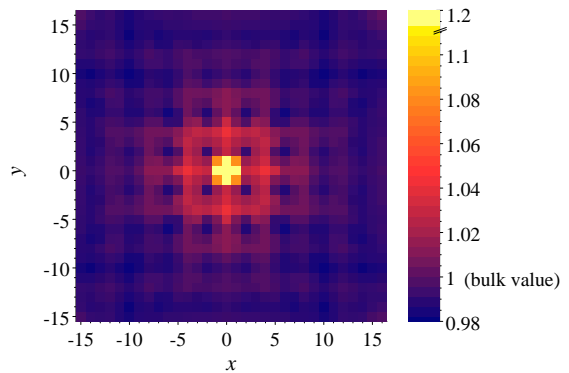


FIG. 3: Grayscale plot of the quasiparticle LDOS in the second model (with all diagrams in Fig 1 summed) near the impurity at lattice site $\mathbf{r}_0 = (0,0)$, measured at $\omega = -0.75\Delta_0$. The parameters of H_{BCS} are as in Fig 2. The SDW fluctuations are characterized by a gap of $\Delta = 5$ meV, $J = 0.15$ eV and a velocity of $c = 0.2$ eV; the SDW-fermion couplings is $\gamma = 0.1$ eV and the pinning strength is $\zeta = 0.4$ eV. A similar modulation occurs for all energies $-2\Delta_0 < \omega < -\Delta_0/8$, and significantly weaker at positive bias $\Delta_0/8 < \omega < 2\Delta_0$.

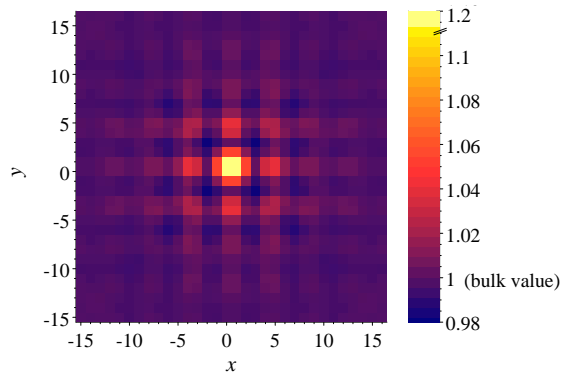


FIG. 4: As in Fig. 3, but now with a plaquette-centered defect at $\mathbf{r}_0 = (0.5, 0.5)$.

were controlled by the susceptibilities $\chi_{\varphi_{x,y}}(\mathbf{k}, \omega_n) = J/(\omega_n^2 + \omega_{x,y}(\mathbf{k})^2)$, where the dispersion $\omega_{x,y}(\mathbf{k})^2 = \Delta^2 + c^2 \min(|\mathbf{k} + \mathbf{K}_{sx,y}|, |\mathbf{k} - \mathbf{K}_{sx,y}|)^2$ [17]. An important difference in this model is that the pinning term is now $-\zeta \int d\tau [\varphi_{x\alpha}^2(\mathbf{r}_0, \tau) + \varphi_{y\alpha}^2(\mathbf{r}_0, \tau)]$, with ζ real; in terms of the previous formulation, this includes both $|\Phi_{x,y\alpha}|^2$ and $\Phi_{x,y\alpha}^2$ terms with equal modulus coefficients. This equality is a weakness of this second model because [6] the physical origin of the two terms is very different, and $|\Phi_{x,y\alpha}(\mathbf{r}_0)|^2$ is better accounted for by a shift in the local spin exciton frequency.

Examples of the spatial dependence of the LDOS of this model are shown in Figs. 3 and 4. Substantial Fourier components at \mathbf{K}_{cx} , \mathbf{K}_{cy} were present at low positive and negative bias. These results are similar to Ref. 5, but the registry of the observed modulations to the underlying Cu lattice is not (yet) known, and this is

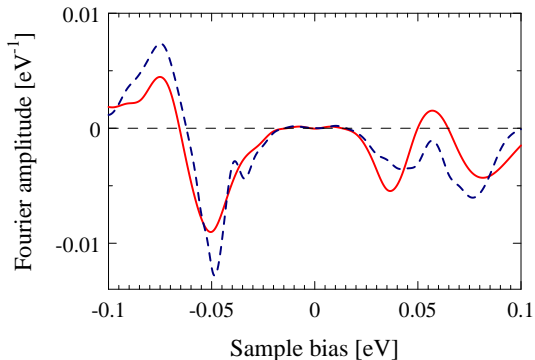


FIG. 5: As in Fig 2 but in the second model with all the diagrams in Fig 1 summed. The solid line is for the parameters in Fig. 3, while the dashed line is for $\gamma = 0.14$ eV, $\zeta = 0.2$ eV. This result depends slightly on the system size (here 32×32 sites) used in the numerical calculation because of the slow decay of the LDOS modulation. The peaks at $\approx \pm\Delta_0 = 0.04$ eV are robust features of the theory, while the structures at other energies depends upon the details of the band structure and position of van Hove singularities.

required for a more precise comparison.

We also used the second model to compute (5) and the results are shown in Fig. 5. A robust feature of the results in Figs 2 and 5 are the peaks in the modulus of the $\mathbf{K}_{cx,y}$ Fourier component near $\pm\Delta_0$. The remaining structure is influenced by both the size of the spin gap, Δ , and the couplings ζ, γ (for a small range of ζ values, multiple defect scattering processes can lead to a local low-energy bound state in the SDW propagator), and depends strongly on the fermionic band structure, $\varepsilon_{\mathbf{k}}$. The van Hove singularities will be attenuated by a finite quasiparticle lifetime. There are also some differences between the two models in Figs 2 and 5 at small values of the spin gap Δ : these are due to the different pinning terms near \mathbf{r}_0 discussed earlier, along with the modification in the bulk fermion spectrum associated with the first diagram on the r.h.s. of Fig 1 which was included only in Fig 5.

This paper has presented a simple theory of the pinning of dynamic SDW fluctuations. Using the dynamic spin susceptibility (as measured in inelastic neutron scattering) and the quasiparticle dispersion as input, we predict the energy dependence of the LDOS at the charge ordering wavevector, as in Figs 2 and 5. We hope that our method will ultimately allow a quantitative comparison of the spectroscopy by inelastic neutron scattering and by STM, and any possible disagreements should help expose physical effects not covered by our simple model.

While this paper was being completed, two related preprints appeared. Zhu *et al.* [18] (like Ref. [16]) discussed static magnetic order in the vortex core, in contrast to our model of dynamic SDW. Howald *et al.* [19] reported STM measurements on $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$

in zero field, including measurements of the energy dependence of the LDOS at the wavevector $(\pi/2, 0)$; the analogous quantity for the charge order nucleated by an impurity is computed here in Figs 2 and 5, and the experimental results at energies around and below Δ_0 are similar to those in Fig 2 for the smaller values of Δ .

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