

Superfluid Density of Strongly Underdoped Cuprate Superconductors from a Four-Dimensional XY Model

M. Franz and A. P. Iyengar

Department of Physics and Astronomy, University of British Columbia, Vancouver, BC, Canada V6T 1Z1
(Received 27 April 2005; published 3 February 2006)

A new phenomenology is proposed for the superfluid density ρ_s of strongly underdoped cuprate superconductors based on recent data for ultraclean single crystals of $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$. We show that the puzzling departure from Uemura scaling and the decline of the slope as the $T_c = 0$ quantum critical point is approached can be understood in terms of the renormalization of quasiparticle effective charge by quantum fluctuations of the superconducting phase. We then employ a $(3 + 1)$ -dimensional XY model to calculate, within particular approximations, the renormalization of ρ_s and its slope, explain the new phenomenology, and predict its eventual demise close to the quantum critical point.

DOI: 10.1103/PhysRevLett.96.047007

PACS numbers: 74.20.-z, 74.25.Fy, 74.72.-h, 74.81.Fa

The manner in which superconductivity in high- T_c cuprates gives way to Mott insulating behavior is a longstanding puzzle of fundamental importance. The anomalous behavior is revealed most strikingly in studies of the doping (x) and temperature (T) dependence of the superfluid density ρ_s [1,2]. As the doping is reduced, both ρ_s and the critical temperature T_c decline while the maximum superconducting gap Δ_0 increases. This dichotomy, along with the empirical Uemura relation $T_c \propto \rho_s$ [3], led to suggestions by numerous authors [4–8] that the superconducting transition in the underdoped cuprates is a *phase-disordering* transition and the pseudogap state [9] above T_c should be thought of as a “phase-disordered” d -wave superconductor. Experiments indeed show evidence for magnetic vortices [10], strong fluctuation diamagnetism [11], and fermionic nodal quasiparticles [12] in the pseudogap state of high- T_c compounds. In addition, there is credible evidence that the superconducting transition in many compounds is in the 3D-XY universality class [13–16] with a wide critical region, exactly as one would expect near a phase-disordering transition.

The focus of the present Letter is to obtain a theoretical understanding of the behavior of ρ_s in *strongly* underdoped cuprates. Theoretical efforts to date have overwhelmingly addressed the phenomenology summarized by Lee and Wen [2]. However, recent experiments performed in unprecedented proximity to the Mott insulator in ultraclean single crystals of $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ (YBCO) [17–19] and in high quality films [20] are quietly overturning the old paradigm: (i) Unlike optimally doped and weakly underdoped samples, the strongly underdoped data show no visible 3D-XY critical region in samples with $T_c \lesssim 25$ K; rather, the approach to T_c is mean-field-like. (ii) Measurements indicate a relationship between the critical temperature and the $T = 0$ superfluid density of the form

$$T_c \propto \rho_s^\gamma, \quad \text{with } \gamma \simeq 0.4\text{--}0.7, \quad (1)$$

a significant departure from the Uemura scaling. (iii) The overall doping and temperature dependence can be pa-

rametrized as

$$\rho_s(x, T) \simeq Ay^2 - By(k_B T), \quad (2)$$

where $y = T_c(x)/T_c^{\text{max}}$ is a measure of the doping x , $T_c^{\text{max}} = 93$ K is the maximum critical temperature for YBCO, $A \simeq 66$ meV, and $B \simeq 9.5$. The demise of superconducting order described by Eq. (2) signals a profound departure from predictions of resonating-valence-bond-type theories and earlier parametrizations of $\rho_s(x, T)$ [2,21]. In what follows, we demonstrate how this new phenomenology follows simply and elegantly from an effective theory describing a phase-fluctuating d -wave superconductor.

The absence of any visible 3D-XY fluctuation region in the data is surprising, since one would naively expect phase fluctuation effects to become more pronounced in the underdoped region as the system approaches the Mott insulator. Upon closer inspection, however, one finds that the observed behavior is entirely consistent with the behavior of a system approaching a quantum critical point [22,23]. Indeed, the $T_c(x)$ line in Fig. 1 must terminate at a quantum critical point (QCP), which by continuity must be in the universality class of the $(3 + z)$ -dimensional XY model, the imaginary time τ providing the extra z dimen-

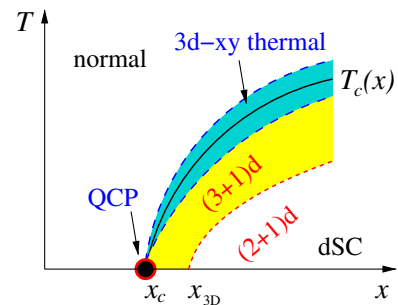


FIG. 1 (color online). Behavior expected in the vicinity of the $(3 + z)$ D-XY quantum critical point in the doping-temperature plane. Solid line $T_c(x)$ represents the superconducting phase transition; dashed lines are crossovers.

sions ($z \geq 1$ being the dynamical critical exponent). Since $D = 4$ is the upper critical dimension for XY -type models, our QCP sits either right at ($z = 1$) or above ($z > 1$) its upper critical dimension, and, thus, we expect *mean-field* critical behavior, possibly with unimportant logarithmic corrections if $z = 1$ [22,23]. As indicated in Fig. 1, when crossing the finite-temperature transition close to the QCP, one still encounters the classical fluctuation region, but its width is now much reduced, and it is likely invisible in experiments.

There is a simple consistency check for the above scenario. If the underdoped region is indeed controlled by the $(3+z)$ D- XY point, then there exists a simple scaling relation between $T_c(x)$ and $\rho_s(x, 0)$ which reads [22,24]

$$T_c \propto \rho_s^{z/(d-2+z)}. \quad (3)$$

For $d = 2$, we recover the Uemura scaling, irrespective of the value of z . In $d = 3$, as appears to be the case in YBCO, we get $T_c \propto \rho_s^{z/(1+z)}$, consistent with the experimental observation of Eq. (1), if $1 \leq z \leq 2$.

It would thus appear that general arguments based on the proximity of the underdoped cuprates to a putative $(3+z)$ D- XY QCP naturally explain items (i) and (ii) in the foregoing list. The scaling analysis leading to Eq. (3), however, holds only when the “bare” parameters of the theory describing the critical degrees of freedom exhibit no significant temperature dependence. In cuprates, quasiparticles in the vicinity of d -wave nodes give rise to a linear temperature dependence in ρ_s which is likely to modify the scaling. In order to address this issue and item (iii), one needs to go beyond the general scaling arguments and consider a specific model. In the rest of the Letter, we formulate and study a particular version of the quantum XY model. We show that, when nodal quasiparticles are included through the effective parameters of this model, it leads to a phenomenology that is consistent with the data.

The simplest model showing the XY -type critical behavior is given by the Hamiltonian

$$H_{XY} = \frac{1}{2} \sum_{ij} \hat{n}_i V_{ij} \hat{n}_j - \frac{1}{2} \sum_{ij} J_{ij} \cos(\hat{\varphi}_i - \hat{\varphi}_j). \quad (4)$$

Here \hat{n}_i and $\hat{\varphi}_i$ are the number and phase operators representing Cooper pairs on site \mathbf{r}_i of a cubic lattice and are quantum mechanically conjugate variables, $[\hat{n}_i, \hat{\varphi}_j] = i\delta_{ij}$. The sites \mathbf{r}_i do not necessarily represent individual Cu atoms; rather one should think in terms of a “coarse grained” lattice model valid at long length scales where microscopic details no longer matter. Classical [25,26] and quantum [24,27] versions of the XY model have been employed previously to study phase fluctuations in the cuprates.

The first term in H_{XY} describes interactions between Cooper pairs; we take

$$V_{ij} = U\delta_{ij} + (1 - \delta_{ij}) \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}. \quad (5)$$

The second term in H_{XY} represents the Josephson tunneling of pairs between the sites; $J_{ij} = J$ for nearest neighbors along the a and b directions, J' along c , and 0 otherwise. In the absence of interactions, J clearly must be identified as the physical superfluid density. We thus take

$$J = J_0 - \alpha T, \quad (6)$$

with $\alpha = (2 \ln 2 / \pi) v_F / v_\Delta$, as in a BCS d -wave superconductor. The T -linear term describes suppression of the mean-field superfluid stiffness by nodal excitations.

On a qualitative level, the physics of the quantum XY model (4) can be understood in terms of the competition between the fluctuations in the local phase $\hat{\varphi}_i$ and charge \hat{n}_i . These are constrained by the uncertainty relation $\Delta\varphi_i \cdot \Delta n_i \geq 1$, which implies that interactions, which tend to localize charge, also necessarily promote phase fluctuations, which then erode the superfluid density. Ultimately, for sufficiently strong V_{ij} , a superconductor-insulator (SI) transition takes place. Charge becomes localized, and an insulating pair Wigner crystal is formed [28]. The latter can be viewed as a superconductor with completely disordered phase. In the rest of the Letter, we assume that the strength of interactions *increases* with underdoping and use V_{ij} to tune our model across the SI transition.

To gain quantitative insight into the behavior of ρ_s in the XY model (4), we employ two complementary approaches: the self-consistent harmonic approximation (SCHA) [25,27], valid for weak interactions, and an expansion in the small order parameter [29,30], valid for strong interactions in the vicinity of the SI transition.

In the SCHA, one replaces H_{XY} by the “trial” harmonic Hamiltonian

$$H_{\text{har}} = \frac{1}{2} \sum_{ij} \hat{n}_i V_{ij} \hat{n}_j + \frac{1}{2} \sum_{\langle ij \rangle} K_{ij} (\hat{\varphi}_i - \hat{\varphi}_j)^2. \quad (7)$$

The constants $K_{ij} = K(K')$ are identified as the renormalized ab -plane (c -axis) superfluid densities [25] and are determined from the requirement that $E_{\text{har}} \equiv \langle H_{XY} \rangle_{\text{har}}$ be minimal. The cuprates are characterized by small values of the anisotropy ratio $\eta = J'/J$. Anisotropy essentially interpolates between the cases $d = 2$ and $d = 3$ and, thus, profoundly affects the approach to the *thermal* phase transition. However, for the quantum phase transition, the effect is very weak. We illustrate this point below by solving the limiting cases $\eta = 1$ (isotropic 3D superconductor) and $\eta = 0$ (decoupled 2D layers) analytically and the intermediate case $0 < \eta < 1$ numerically.

The trial Hamiltonian H_{har} is quadratic in \hat{n}_i and $\hat{\varphi}_j$ and can, thus, be easily diagonalized,

$$H_{\text{har}} = \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} \left(a_{\mathbf{q}}^\dagger a_{\mathbf{q}} + \frac{1}{2} \right), \quad \hbar\omega_{\mathbf{q}} = 2\sqrt{KZ_{\mathbf{q}}V_{\mathbf{q}}}. \quad (8)$$

where $V_{\mathbf{q}}$ is a Fourier transform of V_{ij} and $Z_{\mathbf{q}} = \sum_{\mu=1}^d \sin^2(q_{\mu}/2)$, $d = 2, 3$. For short range interactions $V_{\mathbf{q}} \rightarrow \text{const}$ as $q \rightarrow 0$; we have $\omega_{\mathbf{q}} \sim q$, i.e., an acoustic phase mode. For Coulomb interactions, $V_{\mathbf{q}} \sim 1/q^2$ as $q \rightarrow 0$; we have $\omega_{\mathbf{q}} \rightarrow \omega_{\text{pl}}$, i.e., a gapped plasma mode. Simple power counting then shows that at low T the contribution from the phase mode to the superfluid density is

$$\delta\rho_s^{\text{ph}} \sim \begin{cases} T^{d+1}, & \text{short range interaction} \\ e^{-\omega_{\text{pl}}/T}, & \text{Coulomb interaction.} \end{cases} \quad (9)$$

In either case, the low- T behavior of ρ_s will be dominated by the quasiparticle contribution included via Eq. (6). However, as we demonstrate below, *quantum fluctuations* of the phase lead to strong renormalizations of both the $T = 0$ amplitude of ρ_s and the slope α .

Using $\langle \cos(\hat{\varphi}_i - \hat{\varphi}_j) \rangle_{\text{har}} = \exp[-\frac{1}{2}\langle (\hat{\varphi}_i - \hat{\varphi}_j)^2 \rangle_{\text{har}}]$, an identity valid for harmonic Hamiltonians, we obtain

$$E_{\text{har}} = \langle H_{XY} \rangle_{\text{har}} = \sqrt{KS} - J e^{-\sqrt{S/K}}, \quad (10)$$

with the parameter $\sqrt{S} = (2dN)^{-1} \sum_{\mathbf{q}} \sqrt{V_{\mathbf{q}} Z_{\mathbf{q}}}$ describing the aggregate strength of interactions. Minimizing E_{har} with respect to K , we find

$$K = J e^{-\sqrt{S/K}} \quad (11a)$$

$$\approx J(1 - \sqrt{S/J}), \quad (11b)$$

where the last expression approximates the exact solution over much of the regime of interest [see inset in Fig. 2(a)]. The exact solution of Eq. (11a) exhibits a first order transition at $S \approx 0.541J$. This is an artifact of the SCHA; close to the transition, phase fluctuations become of the order of $\pi/2$, and the harmonic Hamiltonian (8) is no longer a legitimate approximation to H_{XY} . Below, we devise an interpolation formula based on Eq. (11b) that will represent an acceptable solution everywhere except very close to the SI transition.

To obtain the leading temperature dependence, we substitute $J = J_0 - \alpha T$ into Eq. (11b) and expand to leading order in T :

$$\rho_s(x, T) \approx J_0(1 - \sqrt{S/J_0}) - \alpha T(1 - \frac{1}{2}\sqrt{S/J_0}). \quad (12)$$

This is our main result. As expected, both the amplitude and the slope are reduced by quantum fluctuations. Crucially, we observe that the $T = 0$ amplitude decays *faster* than the slope. In particular, for $\sqrt{S/J_0}$ not too large, the above expression is consistent with the experimentally observed behavior Eq. (2) if we identify $y \approx (1 - \frac{1}{2}\sqrt{S/J_0})$. In the language of Ref. [21], the parameter y can be interpreted as the quasiparticle charge renormalization factor.

If we follow Lee and Wen [2] and determine T_c as the temperature at which the superfluid stiffness vanishes, then Eq. (12) implies, to leading order, that $\rho_s(x, 0) \sim T_c^2$, in agreement with the empirical relation Eq. (1). The agreement with the scaling result (3) is, however, entirely co-

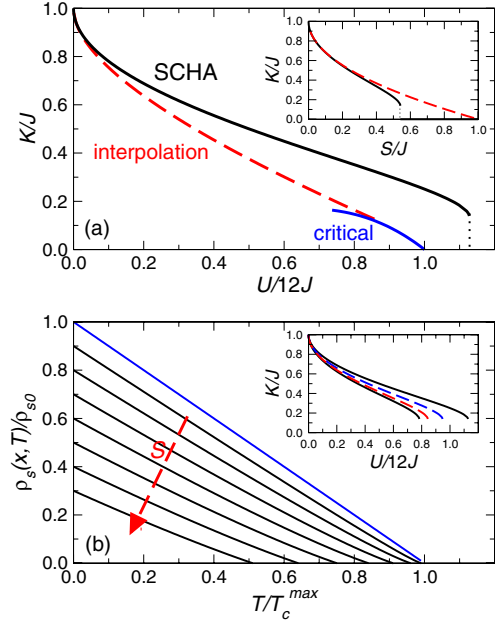


FIG. 2 (color online). Panel (a) shows the SCHA result, the critical theory Eq. (14), and the interpolation discussed in the text (dashed line) for the case $d = 3$ with short range interactions. Inset: The solid line is the exact solution of Eq. (11a), and the dashed line is its approximation Eq. (11b). Panel (b) displays $\rho_s(x, T)$ from Eq. (11b) for several values of S . The inset illustrates the effect of anisotropy: The curves (bottom to top) correspond to $\eta = 0.0, 0.3, 0.6, 1.0$. Solid lines are solutions of Eq. (11a) for $d = 2, 3$ and short range interaction (we find $S/U \approx 0.040$ for $d = 3$ and $S/U \approx 0.058$ for $d = 2$). Dashed lines are numerical solutions of the corresponding anisotropic equations.

incidental since our description of the superfluid density in the SCHA involves an interplay between nodal quasiparticles and *noncritical* quantum phase fluctuations.

For arbitrary anisotropy $0 < \eta < 1$, the SCHA yields a pair of equations for K and K' with structure similar to Eq. (11a). These are easily solved numerically [31], and we give some representative results in the inset in Fig. 2(b). Inspection of this data reveals that all the characteristic features of the $d = 2, 3$ limiting cases remain in place for general anisotropy. For realistic anisotropies $\eta = 10^{-2} - 10^{-3}$, the results become practically indistinguishable from the $d = 2$ case.

In the regime of *strong* fluctuations, it is useful to consider the grand canonical partition function for H_{XY} expressed in the path-integral representation as a trace over Bose field $\varphi_i(\tau)$, $Z = \int \mathcal{D}\varphi \exp(-S/\hbar)$, with the action

$$S = \frac{1}{2} \int_0^\beta d\tau \sum_{ij} [\dot{\varphi}_i V_{ij}^{-1} \dot{\varphi}_j - J_{ij} \cos(\varphi_i - \varphi_j)]. \quad (13)$$

Following Refs. [29,30], we introduce an auxiliary complex field $\psi_i(\tau)$ to decouple, via the familiar Hubbard-Stratonovich transformation, the cosine term in the above action. For short range interaction, the decoupled action is

local in the $\varphi_i(\tau)$ field and the $\mathcal{D}\varphi$ functional integral can be performed *exactly*, to any order in powers of ψ and its derivatives. The field ψ assumes the role of the order parameter of the SI transition. Keeping only terms up to $|\psi|^4$ and replacing the spatial lattice by the continuum yields the desired field-theoretic representation $Z = \int \mathcal{D}\psi \exp(-\mathcal{S}_{\text{eff}}/\hbar)$, where

$$\mathcal{S}_{\text{eff}} = \int d\tau d^d x \left[r|\psi|^2 + \frac{u}{2}|\psi|^4 + \frac{1}{2}|\nabla\psi|^2 + \frac{1}{2c^2}|\partial_\tau\psi|^2 \right],$$

and $r = (d/a_0^2)(1 - 4dJ/U)$, $u = (7da_0^{d-4}/8)J^2(4d/U)^3$, and $c^2 = (4da_0^2/3)(U/4d)^3/J$, with a_0 the lattice spacing.

The above action \mathcal{S}_{eff} predicts a second order SI transition when r changes sign, i.e., when $U = U_c = 4dJ$. Anisotropy again interpolates smoothly between the limiting cases [31] and gives $U_c = 4(2 + \eta)J$. In $(3 + 1)$ dimensions, we expect mean-field theory to work near this transition. In particular, the superfluid density will be given by the saddle-point value of the order parameter $|\psi_0|^2 = -r/u$, which yields

$$\rho_s(x, T) = \frac{8}{7} \left(\frac{U}{12J} \right)^2 (J - U/12), \quad (14)$$

with J given by Eq. (6) and doping parametrized by U . The Coulomb interaction can also be incorporated in \mathcal{S}_{eff} by introducing a gauge field, but the analysis near the critical point of the resulting action is more involved [30] and beyond the scope of this Letter.

The main panel in Fig. 2(a) combines Eq. (14) with the SCHA result adapted to the case of a short range interaction, for which $S = 0.48(U/12)$. The actual solution must interpolate smoothly between SCHA at small $\sqrt{S/J}$ and critical theory near the transition. The dashed line represents an empirical extension of Eq. (11b) to $K = J[1 - \sqrt{S/J} - \lambda(S/J)]$, with $\lambda = 0.625$, which we expect to be very close to the exact solution, as can be verified by quantum Monte Carlo or a similar technique. This interpolation still exhibits the leading behavior of Eq. (12), consistent with experimental data [17–20] as summarized by Eq. (2).

Our results, thus, lend further support to the picture of underdoped cuprates as superconductors with a large pairing gap scale but superfluid stiffness that is severely suppressed by Mott physics. In our approach, the latter is modeled by the charging energy terms in the XY Hamiltonian (4) which significantly renormalize both the $T = 0$ amplitude of the superfluid density $\rho_s(x, T)$ and the quasiparticle effective charge reflected by the slope of its T -linear term. A key new observation of this work is that the systematics of these renormalizations matches that found in underdoped cuprates. In particular, the suppression of the amplitude is *faster* than that of the slope, in agreement with the experimental data [17–20] summarized in Eq. (2). As illustrated in Fig. 2, this behavior persists over a wide range of interaction strengths. Close to the SI transition, the critical theory \mathcal{S}_{eff} takes over. In

this regime, $\rho_s(x, T)$ is given by Eq. (14), which implies that the slope of the T -linear term stops decreasing and, in fact, begins to increase. Thus, our model offers a testable prediction that very close to the SI transition the phenomenology of Eq. (2) will ultimately break down. While the quantitative details of these predictions depend on the specifics of our model and the approximations employed, the general features are controlled by the symmetry and dimensionality and should be robust.

The authors are indebted to I. Affleck, P. W. Anderson, A. J. Berlinsky, D. M. Broun, D. A. Bonn, W. N. Hardy, I. F. Herbut, A. J. Millis, J. Moore, A. Paramekanti, S. Sachdev, and Z. Tešanović for stimulating discussions and correspondence. This work was supported by NSERC, CIAR, and the A. P. Sloan Foundation.

-
- [1] W. N. Hardy *et al.*, Phys. Rev. Lett. **70**, 3999 (1993).
 - [2] P. A. Lee and X.-G. Wen, Phys. Rev. Lett. **78**, 4111 (1997).
 - [3] Y. J. Uemura *et al.*, Phys. Rev. Lett. **62**, 2317 (1989).
 - [4] V. J. Emery and S. A. Kivelson, Nature (London) **374**, 434 (1995).
 - [5] M. Randeria, cond-mat/9710223.
 - [6] M. Franz and A. J. Millis, Phys. Rev. B **58**, 14 572 (1998).
 - [7] L. Balents, M. P. A. Fisher, and C. Nayak, Phys. Rev. B **60**, 1654 (1999).
 - [8] M. Franz and Z. Tešanović, Phys. Rev. Lett. **87**, 257003 (2001).
 - [9] T. Timusk and B. W. Statt, Rep. Prog. Phys. **62**, 61 (1999).
 - [10] Z. A. Xu *et al.*, Nature (London) **406**, 486 (2000).
 - [11] Y. Wang *et al.*, Phys. Rev. Lett. **95**, 247002 (2005).
 - [12] M. Sutherland *et al.*, Phys. Rev. Lett. **94**, 147004 (2005).
 - [13] M. B. Salamon *et al.*, Phys. Rev. B **47**, 5520 (1993).
 - [14] S. Kamal *et al.*, Phys. Rev. Lett. **73**, 1845 (1994).
 - [15] V. Pasler *et al.*, Phys. Rev. Lett. **81**, 1094 (1998).
 - [16] K. D. Osborn *et al.*, Phys. Rev. B **68**, 144516 (2003).
 - [17] T. Pereg-Barnea *et al.*, Phys. Rev. B **69**, 184513 (2004).
 - [18] R. Liang *et al.*, Phys. Rev. Lett. **94**, 117001 (2005).
 - [19] D. M. Broun *et al.*, cond-mat/0509223.
 - [20] Y. Zuev, M. S. Kim, and T. R. Lemberger, Phys. Rev. Lett. **95**, 137002 (2005).
 - [21] A. J. Millis, S. M. Girvin, L. B. Ioffe, and A. I. Larkin, J. Phys. Chem. Solids **59**, 1742 (1998); L. B. Ioffe and A. J. Millis, *ibid.* **63**, 2259 (2002).
 - [22] A. J. Millis, Phys. Rev. B **48**, 7183 (1993).
 - [23] S. Sachdev, *Quantum Phase Transitions* (Cambridge University Press, Cambridge, England, 1999).
 - [24] I. F. Herbut and M. J. Case, Phys. Rev. B **70**, 094516 (2004).
 - [25] E. Roddick and D. Stroud, Phys. Rev. Lett. **74**, 1430 (1995).
 - [26] E. W. Carlson *et al.*, Phys. Rev. Lett. **83**, 612 (1999).
 - [27] A. Paramekanti *et al.*, Phys. Rev. B **62**, 6786 (2000).
 - [28] Z. Tešanović, Phys. Rev. Lett. **93**, 217004 (2004).
 - [29] S. Doniach, Phys. Rev. B **24**, 5063 (1981).
 - [30] M. P. A. Fisher and G. Grinstein, Phys. Rev. Lett. **60**, 208 (1988).
 - [31] A. P. Iyengar and M. Franz (unpublished).