We study a quenched disordered $d = 3 tJ$ Hamiltonian with static vacancies as a model of non-magnetic impurities in high-$T_c$ materials. Using a position-space renormalization-group approach, we calculate the evolution of the finite-temperature phase diagram with impurity concentration $p$, and find several features with close experimental parallels: away from half-filling we see the rapid destruction of a spin-singlet liquid phase (analogous to the superconducting phase in cuprates) which is eliminated for $p \geq 0.05$; in the same region for these dilute impurity concentrations we observe an enhancement of antiferromagnetism. The antiferromagnetic phase near half-filling is robust against impurity addition, and disappears only for $p \geq 0.40$.

The electronic properties and phase diagram of high-$T_c$ materials through a $tJ$ Hamiltonian with static vacancies as a model of non-magnetic impurities is the analogue of the superconducting phase in cuprates, and extend it to incorporate quenched randomness. Our results capture the nature of strongly-correlated systems \cite{9,10,11,12}, and extend an approach that has been successfully applied to a variety of other metals (Al, Ga), for the Cu atoms of the CuO$_2$ planes \cite{1}. The interplay between disorder, strong antiferromagnetic correlations in the parent compound, and doped charge carriers, offers a window onto the nature of both the superconducting phase and the normal state above $T_c$. Doping by nonmagnetic ($S = 0$) Zn ions provides one representative example: the most pronounced effect is the rapid destruction of the superconducting phase \cite{1,2}; in YBCO the transition temperature is reduced at a rate of $\sim 15$K/at.% of impurities, so that it takes Zn concentrations of only about 6% to entirely eliminate superconductivity \cite{2}. This is in contrast to the antiferromagnetic phase at half-filling, which requires a far larger Zn concentration (about 40% in LSCO \cite{3}) to completely suppress. The effects in the metallic region above $T_c$ are equally surprising: nuclear magnetic resonance experiments have found that Zn atoms induce local magnetic moments at nearest-neighbor Cu sites \cite{4}, and enhance antiferromagnetic correlations for several lattice spacings around the impurity \cite{2,3}. In lightly hole-doped LSCO there have been observations of an initial increase in the Néel temperature with Zn addition, and even impurity-induced reappearance of long-range antiferromagnetic order \cite{2,3}.

In this letter we model the effects of nonmagnetic impurities in high-$T_c$ materials through a $d = 3 tJ$ Hamiltonian with quenched disorder in the form of static vacancies. We take a position-space renormalization-group approach that has been successfully applied to a variety of strongly-correlated systems \cite{3,10,11,12}, and extend it to incorporate quenched randomness. Our results capture in a single microscopic model some of the major qualitative features of impurity-doping in real materials: the rapid suppression of a spin-singlet liquid phase which is the analogue of the superconducting phase in cuprates, the gradual reduction of the antiferromagnetic phase near half-filling, and the enhancement of antiferromagnetism away from half-filling for small impurity concentrations.

We consider the quenched disordered $tJ$ model on a $d$-dimensional hypercubic lattice,

\begin{eqnarray}
-\beta H &=& \sum_{(ij)} \left\{ -t \sum_{\sigma} \left( c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma} \right) - JS_i \cdot S_j + V n_i n_j + \mu(n_i + n_j) \right\} + \sum_i \mu_i^{\text{imp}} n_i \\
&=& \sum_{(ij)} \left\{ -\beta H_0(i,j) + \sum_i \mu_i^{\text{imp}} n_i \right\}.
\end{eqnarray}

The first four terms in the Hamiltonian, with $V/J = 1/4$, give the standard $tJ$ model. The static impurities, included through the last term, at each site $i$, occur with probability $p$ via $\mu_i^{\text{imp}} = -\infty$ and do not occur with probability $1 - p$ via $\mu_i^{\text{imp}} = 0$.

To formulate a renormalization-group transformation for this system, we start with simplest case, $d = 1$, and then generalize to $d > 1$ through the Migdal-Kadanoff procedure \cite{13,14}. For $d = 1$ (with lattices sites $i = 1, 2, 3, \ldots$) in principle we could do a partial trace over the degrees of freedom at the even-numbered sites, and map our original system onto a Hamiltonian $-\beta' H'$ depending only on the degrees of freedom at the odd-numbered sites, exactly preserving the partition function. However, since this is a quantum system, the non-commutation of operators in the Hamiltonian means that this decimation can only be carried out approximately \cite{15,16};

\begin{eqnarray}
\text{Tr}_{\text{even}} e^{-\beta H} &=& \text{Tr}_{\text{even}} \sum_i \left\{ e^{-\beta H_0(i,i+1)} + \mu_i^{\text{imp}} n_i \right\} \\
&=& \text{Tr}_{\text{even}} \sum_i \left\{ e^{-\beta H_0(i-1,i+1)} + \mu_i^{\text{imp}} n_i \right\} \\
&=& \prod_i \text{Tr}_i \left[ e^{-\beta H_0(i-1,i+1)} + \mu_i^{\text{imp}} n_i \right] e^{\sum_i \mu_i^{\text{imp}} n_i} \\
&=& \prod_i e^{-\beta' H_0(i-1,i+1)} e^{\sum_i \mu_i^{\text{imp}} n_i} \\
&=& e^{\sum_i \mu_i^{\text{imp}} n_i} e^{-\beta' H'}.
\end{eqnarray}
In the two approximate steps, marked by $\sim$ in Eq. (2), we ignore the non-commutation of operators outside three-site segments of the unrenormalized system. (On the other hand, anticommutation rules are correctly accounted for within the three-site segments, at all successive length scales in the iterations of the renormalization-group transformation.) These two steps involve the same approximation but in opposite directions, which gives some mutual compensation. This approach has been shown to successfully predict finite-temperature behavior in earlier studies [17, 18].

The algebraic content of the renormalization-group transformation is contained in the second and third lines of Eq. (2), yielding the renormalized pair Hamiltonian

$$-\beta H_0(i, j) = -t_{ij} \sum_{\sigma} \left( c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) - J_{ij} S_i \cdot S_j + V_{ij} n_i n_j + \mu_{ij}(n_i + n_j) + \nu_{ij}(n_i - n_j) + G_{ij},$$

where the interaction constants $K_{ij} \equiv (t_{ij}, J_{ij}, V_{ij}, \mu_{ij}, \nu_{ij})$ are nonuniform, and distributed with a joint quenched probability distribution $P(K_{ij})$. This generalized form of the Hamiltonian remains closed under further renormalization-group transformations. Through Eq. (3) we can write the interaction constants $K_{i'j'}$ of the renormalized pair Hamiltonian $-\beta' H_0(i', j')$ as a function of the interaction constants $K_{i'k}$ and $K_{k'j'}$ of two consecutive nearest-neighbor pairs in the unrenormalized system, $K_{i'j'} = R(K_{i'k}, K_{k'j'})$. This function $R$ comes in two varieties, depending on whether or not there is an impurity at site $k$, which we shall denote as $R_0$ and $R_{\text{imp}}$ respectively. Starting with a system with quenched probability distribution $P(K_{ij})$, the distribution $P'(K_{i'j'})$ of the renormalized system is given by the convolution (7):

$$P'(K_{i'j'}) = \int dK_{i'k} dK_{k'j'} \left[ \delta(K_{i'j'} - R_{\text{imp}}(K_{i'k}, K_{k'j'})) \right] \left[ \delta(K_{i'k} - R_0(K_{i'k}, K_{k'j'})) \right].$$

We have thus expressed the renormalization-group transformation for the $d = 1$ system in terms of quenched probability distributions. The initial condition for the renormalization-group flow is the distribution corresponding to the original system in Eq. (1), $P_0(K_{ij}) = \delta(K_{ij} - K_0)$, where $K_0 = \{t, J, V, \mu, 0\}$.

To formulate the renormalization-group transformation for $d > 1$, we employ the Migdal-Kadanoff [13, 14] procedure, which has been widely and successfully applied to both classical and quantum systems (for an overview, see [11]). While approximate for hypercubic lattices, the recursion relations generated by this procedure are exact on hierarchical lattices [17, 18, 19], and we shall use this correspondence to describe the renormalization-group transformation for the case $d = 3$, with length rescaling factor $b = 2$. The associated hierarchical lattice is shown in Fig. 1. Its construction proceeds by taking each bond in the lattice, replacing it by the connected cluster of bonds in the middle of Fig. 1, and repeating this step an infinite number of times. The renormalization-group transformation consists of reversing this construction process, by taking every such cluster of bonds, decimating over the degrees of freedom at the four inner sites of the cluster, yielding a renormalized interaction between the two edge sites of the cluster. Denoting these edge sites as $i', j'$, and the four inner sites as $k_1, \ldots, k_4$, this decimation can be expressed as $K_{i'j'} = \sum_{n=1}^4 R(K_{i'k_n}, K_{k_nj'})$. Just as in the $d = 1$ case, this decimation will give, after a single renormalization-group transformation, a system with a nonuniform quenched distribution of interaction constants. We can calculate the quenched probability distribution $P'(K_{i'j'})$ of the renormalized system through a series of pairwise convolutions. For this purpose we require two types of convolutions: a decimation convolution, defined above in Eq. (4), and a “bond-moving” convolution, using the function $R_{\text{b-m}}(K_A, K_B) = K_A + K_B$. We obtain the renormalized probability distribution $P'$ from the initial distribution $P$ through the following series of pairwise convolutions: (i) a decimation convolution of $P$ with itself, yielding $P_1$; (ii) a bond-moving convolution of $P_1$ with itself, yielding $P_2$; (iii) a bond-moving convolution of $P_2$ with itself, yielding $P'$. In order to numerically implement the convolution, the probability distributions are represented by histograms, where each histogram is a set of interaction constants $(t, J, V, \mu, \nu)$ and an associated probability. Since the number of histograms that constitute the probability distribution increases rapidly with each renormalization iteration, a binning procedure is used [21]: Before every pairwise convolution, the histograms are placed on a grid, and all histograms falling into the same grid cell are combined into a single histogram in such a way that the average and the standard deviation of the probability distribution are preserved. Any histogram within a small neighborhood of a cell boundary is proportionately shared between the adjacent cells. After the convolution, the original number of histograms is retained. Furthermore since evaluation of the $R$ functions is computationally expensive, and most of the weight of the probability distributions is carried by a fraction of the histograms, we have added an additional step before the decimation convolution to increase efficiency: the histograms with the 100 largest probabilities are left unchanged, while the others are collapsed into a single histogram in a way that preserves the average and standard deviation of the...
Let us define a singlet pair-pair correlation function

\[ T_{ij,kl}^{\text{sing}} = \langle \Delta_{ij}^{\text{sing}} \Delta_{kl}^{\text{sing}} + \Delta_{ij}^{\text{sing}} \Delta_{kl}^{\text{sing}} \rangle, \]

where \( \Delta_{ij}^{\text{sing}} = \sqrt{2} (c_{i1} c_{j1} - c_{i1} c_{j1}) \), and the analogous triplet correlation function \( T_{ij,kl}^{\text{trip}} \) in terms of \( \Delta_{ij}^{\text{trip}} = c_{i1} c_{j1} + \frac{1}{\sqrt{2}} (c_{i1} c_{j1} + c_{i1} c_{j1}) + c_{i1} c_{j1} \). For clusters of three consecutive sites \( i, j, k \) in the lattice, Fig. 2 shows the on-site correlations \( T_{ij,ij}^{\text{sing}}, T_{ij,ij}^{\text{trip}}, \) and nearest-neighbor correlations \( T_{ij,kl}^{\text{sing}}, T_{ij,kl}^{\text{trip}} \). In Fig. 3(a) and (b), we see a constant temperature slice at \( 1/t = 0.10 \) as \( \mu/J \) is varied. There is a broad region of chemical potentials away from half-filling, centered at the \( \tau \) phase, where both the on-site and nearest-neighbor singlet correlations are strong, in contrast to the triplet correlations, which are suppressed in the same region. We see similar behavior in Fig. 3(c), where the correlations are plotted as a function of temperature \( 1/t \) at a constant electron density \( \langle n_i \rangle = 0.67 \). As we decrease the temperature, approaching the transition into the \( \tau \) phase, there is a significant increase in the singlet correlations and rapid decay of the triplet correlations. These results point to the possibility that the \( \tau \) phase behaves like a liquid of spin singlets, i.e., a hole-doped resonating valence bond (RVB) state \[ 23, 24 \]. Such a state is expected to superconduct at low enough temperatures. As we shall see below, the effects of impurities on the system are consistent with this RVB interpretation of the \( \tau \) phase.

In Fig. 4 we show the evolution of our calculated phase diagram with increasing impurity concentration \( p \). The \( \tau \) phase is rapidly suppressed for \( p = 0.01 \) through 0.04 [Fig. 4(a)-(d)], and is no longer present by \( p = 0.05 \). The rate at which the \( \tau \) phase disappears is comparable to the reduction of \( T_c \) with nonmagnetic impurities in cuprates, where typically concentrations \( \approx 2-6\% \) (depending on dopant) are enough to eliminate superconductivity \[ 1, 2 \]. As the area of the \( \tau \) phase recedes for these small impurity concentrations, the region it formerily occupied is replaced by a complex lamellar structure of the AF phase. We can understand this enhancement of antiferromagnetism through the RVB picture of the \( \tau \) phase \[ 25 \]; in the pure case the nearest-neighbor singlets resonate in all possible arrangements along the bonds; when an impurity is added some of these arrangements are “pruned”, because the bonds adjacent to the impurity can no longer accommodate singlets. This inhibition of singlet fluctuations leads to enhanced antiferromagnetic correlations around the vacancy. Such lo-
second-order and first-order phase boundaries respectively. Figure 3: On-site and nearest-neighbor singlet and triplet pair-pair correlations for the $p$ concentration $= 0$ constant temperature $1/t = 0.10$. In (c) they are plotted as a function of temperature $1/t$, at the constant electron density $(n_i) = 0.67$. The corresponding phases are indicated near the top of each plot, with solid and dotted vertical lines marking second-order and first-order phase boundaries respectively.

Figure 4: Calculated phase diagrams of the $d = 3$ $tJ$ model, with $p = 0$, $J/t = 0.444$, $V/J = 0.25$, reproduced from Ref. [22]. In (a) and (b) the correlations are plotted as a function of chemical potential $\mu/J$ at constant temperature $1/t = 0.10$. In (c) they are plotted as a function of temperature $1/t$, at the constant electron density $(n_i) = 0.67$. The corresponding phases are indicated near the top of each plot, with solid and dotted vertical lines marking second-order and first-order phase boundaries respectively.

The enhancement of AF phase away from half-filling, which we find at small impurity concentrations, is consistent with previous experimental and theoretical indications.

On the other hand for larger concentrations of impurities, the dilution of the spins in the lattice becomes the dominant effect, and eventually all long-range magnetic order is destroyed in the system. We see this in Fig. 4(e)-(h), showing phase diagrams for $p = 0.10$ through 0.40, and in the inset which plots the AF transition temperature as a function of $p$ near half-filling ($\mu/J = 100$). In contrast to the $\tau$ phase, the AF phase around half-filling is robust against impurity addition, and only disappears for $p \gtrsim 0.40$. This compares favorably to measurements in the half-filled compound La$_2$Cu$_{1-x}$Zn$_x$O$_4$, where Zn
concentrations of $z \approx 0.4$ are required to reduce the Néel temperature to zero [3].

To summarize, we have applied a position-space renormalization-group approach to a quenched disordered $d = 3$ $tJ$ model, and found the evolution of the phase diagram as a function of impurity concentration. The spin-singlet liquid phase away from half-filling is quickly destroyed through the addition of small quantities of static vacancies, while antiferromagnetism in the same region is enhanced. The antiferromagnetic phase near half-filling is less sensitive to impurity addition, and completely disappears only at larger concentrations. These renormalization-group results all have close parallels in experimental results from cuprates.

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