Spin polaron in a magnetic field

D. Veberič1,* P. Prelovšek1,2, and I. Sega1
1 Jozef Stefan Institute, SI-1001 Ljubljana, Slovenia
2 Faculty of Mathematics and Physics, University of Ljubljana, SI-1000 Ljubljana, Slovenia

The influence of the homogeneous magnetic field on a single mobile hole in a magnetic insulator, as represented by the two-dimensional $t$-$J$ model, is investigated by considering the coupling of the field to the orbital current. The energy of the $J = 0$ system is analyzed via the high-temperature expansion and the small system diagonalization. The susceptibility is shown to be diamagnetic and diverging at low temperatures $T$. In contrast, in the antiferromagnetic $J > 0$ case small systems generically reveal a tendency towards a paramagnetic response in larger fields at low $T$. By employing at $T = 0$ the cumulant expansion we study the ground state in arbitrary $B$, showing a behavior very sensitive to the character of the quasiparticle dispersion and the magnetic-field strength. At low $B$ the perturbation and small-systems results are consistent with a pronounced diamagnetic susceptibility at $T \to 0$, but indicate on a suppressed contribution at intermediate $T \sim J$.

PACS numbers: 71.27.+a, 75.20.-g, 74.72.-h

I. INTRODUCTION

In a system of correlated electrons the external magnetic field can induce several interesting effects. Theoretically the least understood are those phenomena, where the magnetic field couples to the motion of charge carriers. In recent years it has been realized that the understanding of the anomalous temperature- and doping-dependence of the Hall effect[1] is one of the most challenging questions in connection with the normal state of cuprates, being representatives of two-dimensional (2D) doped magnetic insulators. Here even the sign of the effect is theoretically controversial[2,3]. The diamagnetic contribution to the d.c. susceptibility has been much less investigated[4], although it is closely related to the Hall conductivity[3]. It emerges from the orbital motion of mobile carriers. For noninteracting electrons the contribution corresponds to the Landau diamagnetism, which is largely temperature independent. In analogy to the Hall effect and other anomalous properties of the normal state in cuprates, one could expect anomalies also in the diamagnetic contribution. So far, however, both experimental and theoretical answers are lacking.

Magnetic field dependence of the eigenstates of tight-binding electrons is nontrivial even in the absence of any electron correlations[5], in particular when the dependence of the ground state on the field strength $B$ and electron density is investigated[6,7]. There have been only few analogous studies of correlated systems. Recently, the ground state of a single hole in the 2D $t$-$J$ model in the presence of magnetic field[8] has been studied. The main message is that for finite (but not very small) $B$ the energy is reduced by an amount proportional to parameter $t$, and the result in such a doped insulator was interpreted in terms of the composite nature of quasiparticles (QP)[9,10]. Another evident observation is, however, the difficulty to extract a reasonable result from studies of small systems.

The aim of this paper is to elaborate on the problem of a single hole in a magnetic insulator in the presence of a homogeneous magnetic field. We study the planar $t$-$J$ model[11] as a prototype model for strongly correlated electrons and electronic properties of cuprates,

\begin{equation}
H = -t \sum_{\langle ij \rangle s} \left( e^{i\theta ij} \tilde{c}_{ij}^\dagger \tilde{c}_{ij} + \text{H.c.} \right) + J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{1}
\end{equation}

where $\tilde{c}_{ij}^\dagger, \tilde{c}_{ij}$ are fermionic operators, projecting out states with the double occupancy. We consider the system in a homogeneous field $B$, perpendicular to the plane, and use for convenience the Landau gauge, where

\begin{equation}
\theta_{ij} = \frac{e}{\hbar} \mathbf{d}_{ij} \cdot \mathbf{A}(\mathbf{r}_i), \quad \mathbf{A} = B(0, x, 0), \tag{2}
\end{equation}

with $\mathbf{d}_{ij} = \mathbf{r}_j - \mathbf{r}_i$. The relevant parameter for the strength of $B$ is the dimensionless flux per plaquette $\alpha = 2\pi B a_0^2 / \phi_0$, where $\phi_0 = h/e$ is the unit quantum flux, and the relevant regime is $\pi < \alpha < \pi$. Further on we set the lattice spacing $a_0 = 1$, as well as $h = k_B = 1$.

In the following we restrict our study of the model Eq. (1) to the case of a single hole doped into a magnetic insulator. The idea is that results for a single hole (spin polaron) remain relevant for the regime of finite, but low, hole concentration $c_h \ll 1$. Here a semiconductor-like picture implies, so that most measurable quantities, assuming the independence of spin polarons, should simply scale with $c_h$. E.g., the diamagnetic susceptibility should behave as $\chi \propto c_h$.

The ground state of the spin polaron at $B = 0$ has been studied extensively both by analytical and numerical approaches, and can be considered as one of few rather settled problems within the theory of correlated systems. Still, here at least two substantially different regimes have to be distinguished.

At finite $J > 0$ (as relevant for cuprates with $J/t \sim 0.3$) the ground state of a hole in an antiferromagnetic (AFM)

1
spin background has the property of a quasiparticle (QP) with $S = 1/2$ and a well defined dispersion $\varepsilon_0(k)$. Consistent results have been obtained for $\varepsilon_0(k)$ using the self-consistent Born approximation (SCBA) [12,13], perturbation expansion [14], numerical approaches including both the exact diagonalization of small systems and the quantum Monte Carlo method [15]. Calculations reproduce a minimum at $k^* = (\pm \pi/2, \pm \pi/2)$, which is very anisotropic, i.e., $\mu = m_\perp/m_\parallel \sim 5$ for $J/t \sim 0.3$. This indicates a very weak dispersion along the AFM zone boundary, connecting $k = k^*$ with $k = k^{**} = (\pi, 0), (0, \pi)$. Studying small systems [14] the latter dispersion is not easy to reproduce correctly. E.g., on a frequently studied system of $4 \times 4$ sites, states with $k^*$ and $k^{**}$ are degenerate, so pronounced finite size effects are expected. Since a small $B$ just probes the effective mass of the QP, it is not surprising that results obtained on small lattices are not reliable or can be even misleading [16]. In another case, ARPES measurements on undoped cuprates [17] show a more isotropic minimum around $k^*$. The explanation seems to be beyond the simple $t$-$J$ model, and the additional effect is attributed to the next-nearest-neighbor hopping ($t'$) term [17].

The behavior at $J = 0$ is quite different. As shown by Nagaoka [18], the ground state is ferromagnetic (FM) with $S = {S_{\text{max}}}$ and momentum $k = 0$, where the QP is a simple hole in the filled band of polarized electrons with an unrenormalized band mass. Nevertheless, close to this simple QP branch there is a large density of complicated excited states, where the hole motion is predominantly incoherent [19]. Therefore it is expected that even moderate temperature $T > 0$ should have a considerable effect.

The paper is organized as follows. Section II is devoted to the study of a single hole at $J = 0$ and arbitrary $B$. Results are obtained via the high-$T$ expansion and the Lanczos diagonalization technique for small systems at $T = 0$ and for $T > 0$ as well. In Sec. III we consider the AFM case with $J > 0$. Here the analysis of small systems at finite $B$ is employed together with the study of the ground state using the cumulant expansion in $t/J$, which has proven to be very informative for $B = 0$ [14]. In the last section, Sec. IV, our results are summarized and a brief discussion on the magnitude of the susceptibility and its relation to the Hall constant is presented.

II. $J = 0$ CASE

A. High-$T$ expansion

To study a single hole, as described by the model Eq. (1) with $J = 0$ and $B > 0$, we first use the standard high-$T$ expansion (HTE). Its application is in this case simple, since the only expansion parameter is $t/T$, while $B$ remains arbitrary. The free energy

$$F = -T \ln Z = -T \ln \text{Tr} e^{-\tilde{\beta} \hat{H}},$$

is within the high temperature expansion expressed in terms of moments $\mu_n$ and cumulants $\lambda_n$

$$\ln Z = \ln \text{Tr} 1 + \ln \left[ 1 + \sum_{n=1}^{\infty} \frac{\beta^n}{n!} \mu_n \right]$$

$$= \ln \text{Tr} 1 + \sum_{n=1}^{\infty} \frac{\beta^n}{n!} \lambda_n,$$

where $\beta = t/T$, $\tilde{\beta} = H/t$ and

$$\mu_n = (-1)^n \text{Tr} \tilde{H}^n / \text{Tr} 1.$$

Moments $\mu_n$ can be expressed as a sum over $(n/2)^2$ closed graphs (paths). Counting different spin configurations for $B = 0$ which remain unchanged [14] after the performed path, each graph contributes a weight $2^{f-r+1}$. Here $f$ is the number of cycles in the spin permutation resulting from a hole traversing the graph, and $r$ is the number of different sites in the graph. For $B > 0$ the only change comes from the contribution of the enclosed magnetic flux, so that the weight becomes

$$w_n = 2^{f-r+1} e^{i m \alpha},$$

where $m$ is the area of the graph in units of $a_0^2$.

Here it is helpful to choose a 45° rotated coordinate system so that a 2D graph decouples into a direct product of two 1D graphs. In this way it is straightforward to generate nonequivalent graphs numerically. We were able to evaluate $\mu_n$ and $\lambda_n$ up to the order $n = 18$. In Table II lowest cumulants $(n \leq 6)$ $\lambda_n = \sum_m \lambda_{nm} \cos m \alpha$ are presented for illustration, while higher cumulants are available upon request.

| $\lambda_{nm}$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 |
|---------------|---|---|---|---|---|---|---|
| 0             | 1 |   |   |   |   |   |   |
| 2             |   | 4 |   |   |   |   |   |
| 4             | -20 | 2 |   |   |   |   |   |
| 6             | 472 | -48 | $\frac{3}{2}$ |   |   |   |   |
| 8             | -24518 | 5992 | -198 | $\frac{3}{2}$ | $\frac{1}{4}$ |   |   |
| 10            | 2207234 | $-\frac{2703635}{4}$ | $\frac{65195}{2}$ | $-\frac{1065}{2}$ | $-\frac{1155}{32}$ | $\frac{5}{8}$ | $\frac{5}{32}$ |
From Eqs. (3,4,5) the series for the orbital susceptibility (per one hole) can be generated,

\[
\frac{\chi}{\chi_0} = \frac{1}{12} \beta^2 + \frac{13}{120} \beta^4 - \frac{2087}{16128} \beta^6 + \frac{8161}{53700} \beta^8 - \cdots,
\]

\[
(\beta) = \int \rho(\varepsilon) e^{-\beta \varepsilon} d\varepsilon,
\]

\[
\mu_n = \int \varepsilon^n \rho(\varepsilon) d\varepsilon,
\]

where \( \chi_0 = \mu_0 e^2 a_0^4 / \hbar^2 \).

There is no unique procedure for the extrapolation of the power series Eqs. (4,5,6) to low \( T \). For the present problem the most reasonable approach seems to be via the density of states \( \rho(\varepsilon) \) and their moments \( \mu_n \),

\[
Z = \int \rho(\varepsilon) e^{-\beta \varepsilon} d\varepsilon,
\]

\[
\mu_n = \int \varepsilon^n \rho(\varepsilon) d\varepsilon.
\]

The density of states can be expanded in terms of Legendre polynomials,

\[
\rho(\varepsilon) = \sum_{\ell=0}^{\infty} B_{\ell} P_{\ell}(\varepsilon), \quad \mu_n = \sum_{\ell=0}^{n} C_{n\ell} B_{\ell},
\]

with coefficients

\[
C_{n\ell} = \frac{\Gamma(\frac{\ell}{2} + \frac{1}{2}) \Gamma(\frac{n}{2} + 1)}{2 \Gamma(\frac{\ell}{2} + \frac{1}{2}) \Gamma(\frac{n}{2} + \frac{1}{2} - \frac{1}{2})},
\]

for \( n > \ell \) and even \( \ell + m \), while \( C_{n\ell} = 0 \) otherwise.

The density of states is used to extrapolate both \( F \) and \( \chi \) to low \( T \). After solving the linear equations (10) for \( B_{\ell} \), we can calculate the susceptibility

\[
\frac{\chi}{\chi_0} = \frac{1}{Z \beta} \left[ \frac{\partial^2 Z}{\partial \alpha^2} - \frac{1}{Z} \left( \frac{\partial Z}{\partial \alpha} \right)^2 \right],
\]

where the same set of equations as in (4,11) holds for derivatives with respect to \( \alpha \) as well.

### B. Small system diagonalization

In analysis of the \( t-J \) model the Lanczos technique for the exact diagonalization of small systems has been already extensively employed [13], predominantly in the investigation of the ground state and their static and dynamic properties. Recently a method combining the Lanczos procedure and the random sampling has been introduced [20] which allows calculation of finite-temperature properties in small correlated systems. The method has been used in the study of various response function within the \( t-J \) model at \( T > 0 \) [20]. The application is particularly simple for static quantities, which can be expressed in expectation values of conserved quantities [21]. The calculational effort is comparable to the ground state evaluation. In particular the average energy \( \langle E \rangle \),

\[
\langle E \rangle \approx \frac{N_{st}}{KZ} \sum_{n=1}^{K} \sum_{m=0}^{M-1} |\langle n|\psi_m^n \rangle|^2 E_m e^{-\beta E_m},
\]

\[
Z \approx \frac{N_{st}}{K} \sum_{n=1}^{K} \sum_{m=0}^{M-1} |\langle n|\psi_m^n \rangle|^2 e^{-\beta E_m},
\]

should be evaluated in this way, where \( |\psi_m^n \rangle, E_m \) are respectively approximate eigenfunctions and energies obtained by the diagonalization within the orthonormal set, generated from the initial functions \( |n \rangle \) in \( M \) Lanczos steps. The \( K \) initial functions \( |n \rangle \) are chosen at random, while \( N_{st} \) is the dimension of the complete basis. Note that it is enough to choose \( M, K \ll N_{st} \). For more detailed explanations we refer to Refs. [20,21].

The introduction of finite \( B > 0 \) in the model, Eq.(1), reduces the translational symmetry and thus for a given system size increases the required minimal basis set. We are at present able to consider the problem of a single mobile hole in canonical 2D systems with \( N = 16, 18, 20 \) sites [22] and periodic boundary conditions (p.b.c.).

It is nontrivial to incorporate phases due to a homogeneous \( B \), being at the same time compatible with p.b.c. It is well known [23] that this can be accomplished only for quantized magnetic fields \( B = mB_0 \), where \( B_0 = \phi_0 / N \) is the smallest field corresponding to the unit quantum flux per system. To incorporate such \( B \) in small systems (tilted squares), the following procedure is used: a) phases \( \theta_{ij} \) for all hops inside squares are left as given within the particular Landau gauge, b) phases attributed to hops across the square boundaries are subject to the condition that the magnetic flux in each plaquette remain the same, i.e. \( B' \equiv B \mod(\phi_0) \) (up to the addition of an unit flux per plaquette). These boundary requirements lead to a set of linear equations which have solutions only for \( B = mB_0 \). Only for an untitled square lattice with \( N = L \times L \) sites the phases can be expressed in a simple form as

\[
\theta_{(i_x,i_y)(i_x,i_y+1)} = Bi_x, \quad \theta_{(i_x,i_y)(i_x+1,i_y)} = 0, \quad i_x < L, \quad \theta_{(i_x,i_y)(1,i_y)} = Bi_y L.
\]

### C. Results

Let us first discuss the polaron internal energy \( \langle \varepsilon(\alpha) \rangle \) as obtained from the high-\( T \) expansion
\[ \langle \varepsilon \rangle = -\frac{\partial (\ln Z)}{\partial \beta} = -t \sum_{n=0}^{\infty} \frac{\tilde{\beta}^n}{n!} \lambda_{n+1}. \]  

(15)

From cumulants \( \lambda_{nm} \) in Table I we see that the \( \alpha \) dependence of \( \langle \varepsilon \rangle \) first enters within the order \( \tilde{\beta}^3 \). Such a term originates from a hole hopping around a loop, contributing to \( \text{Tr} H^4 \) when all spins are equally polarized, in analogy to the processes contributing to the Hall constant \( \tilde{\beta}^3 \). As a result, \( \alpha \) dependence of \( \langle \varepsilon \rangle \) is vanishing fast \((\propto (t/T)^3)\) for \( T > t \).

\[ \Delta \lambda_1 = 1, \]  

as seen in Fig. 1.

It should be observed that for \( N = 16 \) this correction to \( \langle \varepsilon \rangle \) is within the leading order of \( \tilde{\beta}^3 \), while analogous corrections in larger systems, e.g. for \( N = 18 \), emerge only in higher orders. This confirms that on small systems the calculation of \( B \)-induced diamagnetic currents is more delicate than the evaluation of most of the static polaron properties. Nevertheless, at \( J = 0 \) finite size effects are rather well under control, at least in comparison to the AFM case \( J > 0 \) presented in Section III.

Consistency of high-\( T \) expansion and small system \((N > 16)\) results allows reliable extrapolation of the susceptibility \( \chi \) to quite low \( T \sim 0.1 \) \( t \), using the procedure via the density of states \( \rho(\varepsilon) \), Eqs. (9-12). The result is presented in Fig. 2 and as expected \( \chi \) is diamagnetic.

While for \( T >> t \) the susceptibility \( \chi \) is proportional to \( \beta^3 \), the variation is less steep for \( 0.1 \) \( t < T < t \), where the variation is closer to \( \chi \propto \beta^3 \) with \( \eta < 1 \).

It is quite delicate to approach \( T = 0 \) within the \( J = 0 \) model. The ground state for a single hole is within the sector of maximal total spin \( S = S_{\text{max}} \) \([18]\), however excited states are numerous and close in energy, so that the transition between the regime of an incoherent hole propagation and the regime of the large FM polaron appears to happen at surprisingly low \( T^* / t \sim 0.1 \). This is consistent with the well established fact that the FM-polarized ground state is very sensitive to any change of parameters. The behavior of a single hole is simple only strictly at \( T = 0 \). It is expected that the QP at \( B = 0 \) behaves according to the Nagaoka theorem, i.e. as a free hole with energy \( \varepsilon = -4 \) \( t \) in a filled band of spinless fermions.
Looking only in the sector $S = S_{\text{max}}$, a finite field ($B > 0$) should increase the ground state energy according to the cyclotron frequency, i.e. $\delta \varepsilon \sim eB/m^* = Bt$.

In Fig. 3 we show both the absolute g.s. energy $\varepsilon$ and the lowest energy in the sector $S = S_{\text{max}}$ as calculated within small systems with $N = 16, 18$ and $20$. For the Nagaoka sector $S = S_{\text{max}}$ the behavior is for $\alpha < \pi/4$ clearly of the cyclotron type, while for higher $\alpha$ there are some visible commensurability anomalies identical to the study of spinless fermions in a magnetic field [2]. On the other hand, deviations of the absolute ground state from the naive result are much more pronounced. First, even the smallest $B = B_0$ leads to the instability of the $S = S_{\text{max}}$ state, and the actual spin of the g.s. is $S < S_{\text{max}}$. Nevertheless, $\delta \varepsilon$ remains quite close to the cyclotron value. For higher $B > B_0$ the ground state saturates quite abruptly to lowest spin $S = 1/2$ and g.s. energy $\varepsilon$ is much lower than in the $S = S_{\text{max}}$ case. Note, however, that even an approximate validity of the simple cyclotron-frequency argument, $\delta \varepsilon \propto |B|$, implies a divergent susceptibility $\chi(T \to 0) \to \infty$, as found also from the high-$T$ expansion.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig3}
\caption{Ground state energy $\varepsilon$ (in units of $t$) vs. $\alpha$, obtained via the diagonalization of small systems of different sizes and $J = 0$. Open dots correspond to the lowest-energy state within the sector $S = S_{\text{max}}$.}
\end{figure}

### III. $J > 0$: ANTIFERROMAGNETIC SPIN BACKGROUND

$J > 0$ introduces quite a different QP behavior. At $T = 0$ the spin background corresponds to an AFM with long range order. The ground state of the spin polaron is well understood, and corresponds within the $t$-$J$ model to $S = 1/2$ and $\mathbf{k} = \mathbf{k}^*$, with a weak dispersion along the AFM zone boundary.

At least for weak magnetic fields it is expected that the QP description of the hole is still valid, resulting in a cyclotron motion with the linear-in-field dependence of the QP energy. Such behavior, is questioned by recent small-system diagonalisation results [3]. It should be reminded that results obtained from the exact diagonalisation can be misleading due to finite size effects, if the cyclotron radius is comparable to the linear size of the system. With p.b.c. even more pronounced effects compared to those already discussed for $J = 0$ in Sec. II can be expected. For the AFM case they arise from larger ground state degeneracy, and from the near-degeneracy of the QP dispersion along the AFM zone boundary.

#### A. Cumulant expansion method

At $T=0$ we can consider a QP moving in an ordered AFM by performing the expansion starting in the limit $t/J \ll 1$. Here the standard cumulant-expansion (CE) procedure for the ground-state energy, as first considered by C. Bloch [26], is followed.

The implementation of the method in the zero-field case with a single hole in the $t$-$J$ model has been already given in some detail elsewhere [4]. There the diagonal part of the Heisenberg spin interaction in Eq. (1) has been taken as the unperturbed Hamiltonian $H_0$ and the ground-state energy $\varepsilon_0(k)$, expressed relative to the undoped AFM ground state, has been obtained as a double power series in $u = t/J$ and $\gamma = J_\perp/J$

$$
\varepsilon_0(k) = J \sum_{n,m} a_{n,m}(k) u^{\gamma}(\frac{\gamma}{2})^m,
$$

where the $k$-dependence of the expansion coefficients merely reflects the underlying translational invariance of the problem.

A finite magnetic field breaks the translational invariance of the system, so the above result, obtained from the nondegenerate theory is not valid. Indeed, the unperturbed ground state becomes highly degenerate, allowing for any hole position in an otherwise perfectly Néel-ordered spin state, thus the degenerate perturbation theory must be used. The version of the secular determinant as given in [26] is used, which up to the fourth order in perturbation $H'$ reads

$$
(E - E_0)\delta_{ij} = < i | H' \frac{Q_0}{\eta_0} H' | j > + < i | H' \frac{Q_0}{\eta_0} H' \frac{Q_0}{\eta_0} H' \frac{Q_0}{\eta_0} H' | j > - \sum_\ell < i | H' \frac{Q_0}{\eta_0} H' | \ell > < \ell | H' \frac{Q_0}{\eta_0} H' | j > + \cdots
$$

The (bra)kets denote the set of degenerate states – positions of the hole – with the unperturbed energy $E_0$, whereas $P_0$ and $Q_0$ are the projectors onto this subset of states and its complement, respectively, $H'$ is taken to be the sum of the hopping part and the transverse...
spin part of $H$ in (1), while $\eta_0$ stands for the energy
denominator $E_0 - H_0$. A contribution to the matrix
element $M(i, j) = \langle i | \cdot | j \rangle$ resulting from a particular
process $O_\mu$ involving products of operators as in (18) is
calculated from the associated graph $\Gamma$ in any order
of perturbation expansion. However, as the hole moves
from some initial position $i$ to a final but equivalent posi-
tion $j$ under the action of a particular string of operators
$O_\mu$ along some path, it acquires a definite phase factor
$\theta_{ij}$, depending on the path itself. Two such paths are
depicted in Fig. 4.

In the chosen Landau gauge the phase associated with
any link in the $y$-direction is given by the $x$-coordinate of
that link. Thus, the total phase $\theta_{ij}$ acquired by the hole
along the path $C$, is

$$\theta_{ij}(C) = \int_C A \cdot ds = i_x(j_y - i_y)\alpha + \phi_{ij}(C). \quad (19)$$

Here $\phi_{ij}(C)$ is the phase relative to the initial point at $i$.
Care should be taken of the proper orientation in which
the link is traversed. Thus, referring to Fig. 4, phase
along $C_\mu$ is $\phi = -2\alpha$, whereas along the path $A_\mu$, $\phi = 4\alpha$.

to a definite product of operators of order $r = n + m$
along the path from $i \rightarrow j$ [14].

The secular equation (18) becomes a difference equation
for the on-site amplitudes $f_i$ on a rectangular grid
with $N = L_x \times L_y$ sites

$$\varepsilon f_i = \sum_j M(i, j) f_j,$$

$$M(i, j) = \sum_{n, m} u^{n+\gamma} m \sum_{\delta} \omega_{\mu}(i, j) e^{i\delta(i, j)}, \quad (20)$$

where $i$ and $j$ run only over one sublattice, $M(i, j)$ is a
sum of contributions along different paths $C_\mu$, and the
energy $\varepsilon \equiv \varepsilon(\alpha)$ is again measured with respect to the
g.s. of the undoped AFM state. Referring again to Fig. 4
the paths $C_\mu$ and $A_\mu$ would then first appear in order
$u^{8,4} \gamma^4$ and $u^{0,4} \gamma^2$, respectively.

In the chosen gauge Eq. (18), the system is translation-
ally invariant along the $y$-direction. Thus, the ansatz
$f_i = g_i \exp(i k_y i_y)$ reduces the above equation to a differ-
ence equation in one dimension, where $\ell = i_x$, $\ell = j_x$.

$$\varepsilon g \ell = \sum_{\ell'} \tilde{M}(\ell, \ell') g_{\ell'}, \quad 1 \leq \ell, \ell' \leq L_x,$$

$$\tilde{M}(\ell, \ell') = \sum_{\tau} e^{iQ} \sum_{n, m} u^{n+4} m \sum_{\delta} \omega_{\mu}(\ell' - \ell, \tau) e^{i\phi_{\mu}(\ell' - \ell, \tau)}$$

$$Q = k_y + \alpha\ell, \quad (21)$$

and the summation over $\tau$ is restricted to run over values
for which $\ell' - \ell + \tau$ is even, whereas $k_y \in [0, 2\pi]$. Note
also that $\omega$ and $\phi$ do not depend on the initial point $\ell$,
but only on the path $C$. Taking $\alpha = 2\pi p/L_x$, one can
impose the p.b.c. also in the $x$ direction.

The eigenvalue problem of Eq. (21) is solved numeri-
cally for $L_x \gg \xi$, where $\xi = 13$ is the smallest linear size
of the region visited by the hole, within the order of per-
turbation series here considered. In Fig. 4 we plot the g.s.
energy $\varepsilon$ as a function of $\alpha$ at $J/t = 2$ and the isotropic
exchange $\gamma = 1$, evaluated for $L_x = 128$. A linear-in-field
dependence of $\delta \varepsilon(\alpha) = \varepsilon(\alpha) - \varepsilon(0)$ in Fig. 5 is evident for
small $\alpha$, implying that the hole may still be described
as a QP exhibiting cyclotron motion. However, after the
initial rise an almost monotonic decrease is observed and the
minimum of $\varepsilon(\alpha)$ is achieved for $\alpha = \pi$. The figure
includes also the respective data from exact diagonaliza-
tion for $N = 20$. Although both sets of data do not agree
in detail, which can be partially attributed to the perturba-
tional character of the CE results, the overall behavior is
remarkably similar, including the initial rise in $\delta \varepsilon(\alpha)$
for $N = 20$ and the cusp-like behavior close to $\alpha = \pi/2$.
This holds to a lesser degree for other commensurability
points, e.g. for $\alpha = \pi/4$ and $3\pi/4$.

FIG. 4. The phase increments, defined on the (oriented)
links between two neighboring lattice points, in the Landau
gauge $A = B(0, x, 0)$ along two different paths $C_\mu$ and $A_\mu$
connecting points $i$ and $j$.

We have generated all the paths in order $u^{n+\gamma m}$ with
$(n, m)$ up to (2, 4), (4, 4), (6, 3) and (8, 2). Each con-
tribution to the perturbation series in order $(n, m)$ is
then given by the magnitude $\omega(i, j)$ of the matrix ele-
ment $\langle i | O^{(r)}_\mu | j \rangle$ and the phase $\theta_{\mu}(i, j)$, where $O^{(r)}_\mu$ refers
of the quasiparticle dispersion \( \varepsilon_0(\mathbf{k}) \) at the bottom of the QP band, which is poorly reproduced in small systems. Nevertheless, numerical results establish quite consistently the crossover at \( T \sim T^* \propto J \).

For \( T < T^* \), energy \( \langle \varepsilon(\alpha) \rangle \) shows an overall opposite, i.e., a paramagnetic-like variation with \( \alpha \), as found in \cite{Ref14} and reproduced above within the CE with respect to \( t/J \).

The results in this temperature region are more size dependent. At \( T/t = 0.2 \) in Fig. 5 we can find a maximum for \( \alpha > 0 \) only in systems with \( N = 18, 20 \) sites, while the \( N = 16 \) case shows a different behavior. The deviation within the latter system is due to additional symmetry of the \( 4 \times 4 \) system (hypercube).

B. Small-system results

Using the numerical finite temperature technique described in Sec. IIB and applied to the \( J = 0 \) case the results for \( J > 0 \) are also obtained. In the following we choose \( J/t = 0.4 \), which is close to the situation in cuprates, and consider the contribution of the single hole energy \( \varepsilon = E(N_h=1) - E(N_h=0) \) to the internal energy at \( T = 0 \) and \( T > 0 \) \( \langle \varepsilon \rangle \). First note that for \( T \gg \max(t,J) \), the leading order of the high-\( T \) expansion is independent of \( J \) and in this limit results for \( J = 0 \) and \( J > 0 \) match.

In Fig. 6, the intermediate temperature hole energies \( \langle \varepsilon(\alpha) \rangle \) are evaluated at two different \( T \) within different system sizes. Comparing results with those for \( J = 0 \) in Fig. 5, several conclusions can be reached. At higher \( T/t = 1 \) energies \( \langle \varepsilon(\alpha) \rangle \) for \( J = 0 \) and \( J/t = 0.4 \) are qualitatively similar. As a function of \( \alpha \) both cases correspond approximately to the simple \( \cos \alpha \) variation. It is however evident that finite \( J \) considerably reduces (by a factor \( \sim 4 \)) the total energy span.

Relative to the \( J = 0 \) case it is also clear that finite size effects become more pronounced when approaching the low-\( T \) regime. This is related to the near-degeneracy
degenerate dispersion along the magnetic Brillouin zone boundary.

![Graph](image)

FIG. 7. Ground state energy $\varepsilon(\alpha)$ for $J/t = 0.4$, as calculated on systems of $N = 16, 18, 20$ sites.

Finally, let us present in Fig. 8 results for the orbital susceptibility $\chi(\alpha)$, Eq. (7). For $J = 0$ the calculation is performed via high-$T$ expansion as already discussed in Sec. 2. Since we rely only on discrete values of $\alpha$, the analysis of finite-system data for $J/t = 0.4$ is on the other hand less reliable.

![Graph](image)

FIG. 8. Susceptibility $\chi$ vs. $T/t$ for $J/t = 0.4$, as extracted from small-system data $N = 18, 20$.

Moreover, the variation of $F(\alpha)$ is quite subtle at smallest $\alpha_{\text{min}}$, as evidenced also from $\varepsilon$ in Fig. 6. In Fig. 7 the susceptibility $\chi$ is presented as obtained from Eq. (6), with parabolic fit for $F(\alpha)$ using only $\alpha = 0$ and $\alpha = \alpha_{\text{min}}$. This procedure could be questionable for $T < T^*$, but qualitative behavior is still quite instructive. Relative to the $J = 0$ case, the diamagnetism is suppressed by $J > 0$ at higher $T \gg J$. In an intermediate regime $T \sim J$, susceptibility $\chi$ appears even to change sign, i.e. becomes paramagnetic. Only at low $T < T^*$ a pronounced strongly $T$-dependent diamagnetic response is again observed, consistent with the QP cyclotron motion at $T = 0$. It is an interesting observation that an exact solution of the problem on a single plaquette (at $T > 0$) subjected to an effective staggered AFM field, reproduces qualitative features of Fig. 5.

IV. CONCLUSIONS

Our study shows that the calculation of the effects of finite magnetic field, coupled to orbital motion of electrons, becomes delicate in models of correlated electrons, e.g. within the $t$-$J$ model considered in this work. Results for magnetic observables such as the diamagnetic susceptibility appear to be strongly influenced by finite-size effects, which are hard to overcome in available system sizes. Both for $J = 0$ and $J > 0$ some of deviations appear at ‘commensurate’ values of $\alpha$ within the given system geometry, and are particularly large for $N = 16$. We have shown that it is possible to understand such finite-size effects within the high-$T$ expansion or within the $t/J$ perturbation expansion as a contribution of additional graphs due to p.b.c. Still it is impossible to eliminate them systematically in most interesting physical regimes. These effects lead to a nonmonotonous variation of observables, e.g. $\langle \varepsilon(\alpha) \rangle$, which in turn leads to an enhanced uncertainty in $\chi(T)$.

The $J = 0$ case seems both easier to study and to understand. High-$T$ expansion and small systems show a continuous transition from the high-$T$ regime of incoherent hopping to the Nagaoka state at $T = 0$, with a monotonous increase of the diamagnetic $\chi$. At $T > 0$ where the HTE is reliable the variation of the energy with field $\langle \varepsilon(\alpha) \rangle$ is quite close to a simple cos $\alpha$ form. Nevertheless the asymptotic behavior at low $T$ is not simple to establish, since the nature of low lying states (above the Nagaoka state) is complicated.

The behavior of the AFM $J > 0$ polaron is more involved. While at $T \gg J$ the exchange scale $J$ is not important and results qualitatively follow those for $J = 0$, new physics emerges for $T \lesssim J$. A nearly flat $\langle \varepsilon(\alpha) \rangle$ at intermediate regime $T \sim J$ is quite remarkable, and leads to a vanishing diamagnetic $\chi$ (or even change of its sign). It seems, that here $J > 0$ diminishes and even destroys emerging coherence of QP. Only at lower $T < J$ the coherence is established and the known dynamical picture of a coherent AFM polaron is dominating the behavior in lowest fields $\alpha$. Reliable results are however difficult to obtain even for $T = 0$, since in small systems their variation with $\alpha$ is very sensitive to the system shape, boundary conditions etc. due to the very anisotropic and degenerate QP dispersion.

The CE results are very instructive, but it is not straightforward to make them quantitative for $J < t$. 

8
For \( J > t \), where the CE series converges quite rapidly, there is a clear evidence in weak fields that the QP is exhibiting cyclotron motion. The commensurability effects are quite pronounced and agree with finite-cluster data for large \( J/t > 1 \), see Fig. 3. On the other hand, these effects are not evident in small-system results for \( J/t < 1 \). This non-agreement is attributed in part to specific lattice shapes and p.b.c. The flatness of the dispersion seems to be the main reason for the structureless character of small-system data in the region of small \( J/t < 1 \).

Here we would like to point to the close similarity with the challenging theoretical problem of the Hall effect, which is difficult to approach even for very low doping, e.g. for a single hole \( 22 \). Similarly to the orbital susceptibility the Hall effect emerges due to coupling to orbital currents. The Hall constant is given by \( R_H = \sigma_{xy}/B \sigma^2_{xx} \), where the off-diagonal conductivity \( \sigma_{xy} \) can be related to the orbital susceptibility \( \chi \) as

\[
\sigma_{xy} = B \frac{\partial \chi}{\partial \mu} \frac{\partial \mu}{\partial \mu},
\]

where \( \mu \) is the chemical potential. In our case of very low hole doping, i.e., in the semiconductor-like regime, the susceptibility \( \chi \) scales linearly with \( c_h \); moreover \( \partial c_h/\partial \mu = -\beta c_h \), so that \( \sigma_{xy} \propto \chi \). The high-\( T \) expansion of the Hall constant \( R_H(T) \) (the high-frequency value) is analogous to that of \( \chi(T) \) \( 3 \). On the other hand, crossing the scale \( T \sim J \) remains the challenge, whereby it seems that at this intermediate \( T \) the hole-like \( R_H \) is even reduced with respect to its high-\( T \) value \( 44 \). Experiments \( 1 \) indicate that \( R_H \) recovers for \( T < T^* \), varying strongly with \( T \) and approaches the well known quasiclassical result for \( T \to 0 \) \( 23 \). Note that our results for \( \chi(T) \), Figs. \( 8 \) indicate just on such behavior.

Let us finally comment on the magnitude of the diamagnetic susceptibility. Since we are evaluating the case of a single hole, at low doping \( c_h \ll 1 \) the observable diamagnetic contribution to the susceptibility (per unit cell) should be \( \chi = \zeta c_h \chi_0 \), where \( \zeta \) is dimensionless value, presented in Figs. \( 2 \) and \( 8 \). It is convenient to compare these values to the spin susceptibility (per unit cell) of the planar undoped AFM for \( T < T^* \), where \( \chi_s \sim 4.0 \mu_0 \mu_B / J \) \( 21 \). Setting \( m_t = \hbar^2/2t_0^2 \) the ratio can be expressed as

\[
\frac{\chi}{\chi_s} = K' \zeta c_h \frac{J}{t} \left( \frac{m_e}{m_t} \right)^2 \sim 9.3 c_h \zeta, \tag{24}
\]

with \( K' \sim 4.0 \). To estimate the actual value of \( \chi/\chi_s \) in Eq. (27) we take \( c_h \sim 0.15 \), e.g. as in the ‘optimal’ doping regime, and \( \zeta \sim -0.1 \) in the region \( T < T^* \). This gives \( \chi/\chi_s \sim -0.03 \), which is of the same order of magnitude as the experimentally measured value \( 0 \). Note, however, that below the crossover temperature \( T^* \) \( \zeta \) becomes strongly temperature dependent, as opposed to the usual \( T \)-independent Landau-type diamagnetism in Fermi liquids. Since it is difficult to distinguish different contributions to the actual susceptibility in experiments, it remains to be seen whether such \( T \)-dependent \( \chi \) really appears in cuprates and analogous systems.

**ACKNOWLEDGMENTS**

One of the authors (P.P.) wishes to thank X. Zotos for helpful suggestions concerning the introduction of a magnetic field in small systems.

This work was supported by Ministry of Science and Technology of Slovenia under Project No. J1-6166-0106/97.

* E-mail: darko.veberic@ijs.si

[1] For a review see e.g. N. P. Ong, in *High Temperature Superconductors*, ed. by D. M. Ginsberg (World Scientific, Singapore, 1990), Vol. 2, p. 459.
[2] W. Brinkman and T. M. Rice, Phys. Rev. B 4, 1566 (1971); B. S. Shastry, B. I. Shraiman, and R. R. P. Singh, Phys. Rev. Lett. 70, 2004 (1993).
[3] F. F. Assaad and M. Imada, Phys. Rev. Lett. 74, 3868 (1995).
[4] R. E. Walstedt, R. F. Bell, L. F. Schneemeyer, J. V. Waszczak, and G. P. Espinosa, Phys. Rev. B 45, 8074 (1992); M. Miljak, V. Zlatić, I. Kos, J. D. Thompson, P. C. Canfield, and Z. Fisk, Sol. St. Commun., 85, 519 (1993).
[5] A. G. Rojo, G. Kotliar, and G. S. Canright, Phys. Rev. B 14, 9140 (1993).
[6] D. R. Hofstadter, Phys. Rev. B 14, 2239 (1976).
[7] Y. Hasegawa, P. Lederer, T. M. Rice, and P. B. Wiegmann, Phys. Rev. Lett. 63, 907 (1989).
[8] T. M. Rice, in *Proceedings of the Les Houches Summer School, Session LXVI*, ed. by B. Doucet and J. Zinn-Justin (Elsevier, Amsterdam, 1995), p. 19.
[12] S. Schmitt-Rink, C. Varma, and A. Ruckenstein, Phys. Rev. Lett. 60, 2783 (1988); C. L. Kane, P. A. Lee, and N. Read, Phys. Rev. B 39, 6880 (1989).
[13] G. Martinez and P. Horsch, Phys. Rev. B 44, 317 (1991).
[14] P. Prelovšek, I. Sega, and J. Bonča, Phys. Rev. B 42, 10706 (1990).
[15] For a review, see E. Dagotto, Rev. Mod. Phys. 66, 763 (1994).
[16] B. O. Wells et al., Phys. Rev. Lett. 74, 964 (1995).
[17] M. S. Hybertsen et al., Phys. Rev. B 41, 11068 (1990); T. Tohyama and S. Maekawa, Phys. Rev. B 49, 3596 (1994); A. Nazarenko, K. J. E. Vos, S. Haas, E. Dagotto, and R. J. Gooding, Phys. Rev. B 51, 8676 (1995).
[18] Y. Nagaoka, Phys. Rev. 147, 392 (1966).
[19] W. Brinkman and T. M. Rice, Phys. Rev. B 2, 6880 (1970).
[20] J. Jaklič and P. Prelovšek, Phys. Rev. B 49, 5065 (1994); Phys. Rev. Lett. 74, 3411 (1995); 75, 1340 (1995); Phys. Rev. B 52, 6903 (1995).
[21] J. Jaklič and P. Prelovšek, Phys. Rev. Lett. 77, 892 (1996).
[22] J. Oitmaa and D. D. Betts, Can. J. Phys. 56, 897 (1978).
[23] E. Fradkin, Field Theories of Condensed Matter Systems, (Addison-Wesley, Redwood City, 1991), Frontiers in Physics Vol. 82, p. 252.
[24] M. Kohmoto, Phys. Rev. B 39, 11943 (1989); Y. Hasegawa, Y. Hatsugai, M. Kohmoto, and G. Montambaux, Phys. Rev. B 41, 9174 (1990).
[25] C. Bloch, Nucl. Phys. 6, 329 (1958).
[26] A. Messiah, Quantum Mechanics (Nord-Holland, Amsterdam, 1962), Vol. 2, p. 717.
[27] Note that within the CE approach the g.s. is AFM-like to any finite order of the perturbation series. The hole can thus visit sites of one sublattice only.
[28] P. Prelovšek, Phys. Rev. B 55, 9219 (1997).
[29] R. R. P. Singh and R. L. Glenister, Phys. Rev. B 46, 11871 (1992).