Eur. Phys. J. B **5**, 465–471 (1998)

THE EUROPEAN PHYSICAL JOURNAL B

A microscopic model for the intrinsic Josephson tunneling in high-T_C superconductors*

W. Hanke[1], O. Schmitt[1], H. Endres[1], R. Kleiner[2], and P. Müller[2]

[1] Institut für Theoretische Physik, Universität Würzburg, 97074 Würzburg, Germany
[2] Physikalisches Institut III, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Received: 24 February 1998 / Revised: 28 April 1998 / Accepted: 23 June 1998

Abstract. A quantitative analysis of a microscopic model for the intrinsic Josephson effect in high-temperature superconductors based on interlayer tunneling is presented both within a mean-field BCS evaluation and a numerically essentially exact Quantum Monte-Carlo study. The pairing correlations in the CuO_2-planes are modelled by a 2D Hubbard model with attractive interaction, a model which accounts well for some of the observed features such as the short planar coherence length. The stack of Hubbard planes is arranged on a torus, which is threaded by a magnetic flux. The current perpendicular to the planes is calculated as a function of applied flux (*i.e.* the phase), and – after careful elimination of finite-size effects due to single-particle tunneling – found to display a sinusoidal field dependence in accordance with interlayer Josephson tunneling. Studies of the temperature dependence of the supercurrent reveal at best a mild elevation of the Josephson transition temperature compared to the planar Kosterlitz-Thouless temperature. These and other results on the dependence of the model parameters are compared with a standard BCS evaluation.

PACS. 74.20.-z Theories and models of superconducting state – 74.20.Mn Nonconventional mechanisms (spin fluctuations, polarons and bipolarons, resonating valence bond model, anyon mechanism, marginal Fermi liquid, Luttinger liquid, etc.) – 71.10.Fd Lattice fermion models (Hubbard model, etc.)

1 Introduction

The high-T_C superconductors (HTSC) reveal a number of unusual properties. One unique example, important both from a fundamental and from an applied point of view, is the intrinsic, "microscopic" Josephson effect: a single crystal like $Bi_2Sr_2CaCu_2O_8$ (BSCCO) consists of natural stacks of thousands of Josephson junctions, with the CuO_2 layers acting as superconducting electrodes and the Bi_2O_3 layers as insulating ("intrinsic") barriers, closely packed on a microscopic length scale ($d \approx 1$ Å). This intrinsic Josephson effect was first discovered for BSCCO–[1,2] and later confirmed in YBaCuO–[3] materials. From the point of view of the microscopic theory of the HTSC, this is an important effect for the c-axis transport and possibly the pairing theory. [4–6].

A theoretical description of the intrinsic Josephson current must explain both the Kosterlitz-Thouless-type of superconductivity in the planes [7–10] and the effective coupling of these planes on a microscopic basis. In previous theoretical studies of the intrinsic Josephson effect, the supercurrent was not investigated on such a rigorous microscopic basis. Rather, it was studied using macroscopic electrodynamics employing, for example, empirically derived coupled Sine-Gordon equations for stacked Josephson junctions [11,12].

In this paper, we present numerical evidence based on Quantum Monte-Carlo (QMC) simulations for the existence of the supercurrent and the intrinsic Josephson effect on a purely microscopic basis. The simulated model consists of a stack of coupled Hubbard planes for which, in analogy to the experimental situation, each individual plane is modelled by a two-dimensional (2D) short coherence-length superconductor [8,9,13], *i.e.* the 2D attractive Hubbard model.

The attractive ("negative-U") Hubbard model is the simplest lattice model for correlated electrons which can become superconducting. In 2D it has previously been shown numerically to undergo a Kosterlitz-Thouless transition into a superconducting s-wave state away from half-filling [10]. There are definite similarities between the phase diagram of this simple lattice model and the phase diagram of the cuprate HTSC: both systems exhibit a phase transition along a certain critical line as a function of a particular control parameter, which is the strength of the attractive coupling in case of the Hubbard model and the hole (electron) doping in the CuO_2 planes for the cuprates. Furthermore, both show a remarkable crossover along this phase transition line with similar

* Dedicated to J. Zittartz on the occasion of his 60th birthday

consequences: at one endpoint (underdoped/strong-coupling limit) a pairing description in terms of Bose-Einstein condensation with "pre-formed" pairs is more adequate, with a superconductor to insulator critical endpoint, whereas at the other end (overdoped/weak-coupling regime), a behavior similar to a conventional BCS superconductor results, where the system undergoes a normal metal to superconductor transition.

In the intermediate-coupling regime in 2D, the physics will be dominated by the interplay between quasi-particles and bound pairs, which leads to non-trivial behavior: some basic physical features characterizing this regime have previously been studied by numerical means, which showed important deviations from canonical Fermi-liquid theory [7].

This last point is particularly interesting also in view of work by Anderson and coworkers [4–6], where it is argued that the unusual c-axis resistivity data obtained for cuprate superconductors are the result of the non-Fermi liquid nature of the in-plane (CuO_2) ground state of these materials. This non-Fermi liquid nature is taken as responsible for disrupting the interplane hopping of electrons so strongly that single electrons effectively do not hop between the planes, giving rise to anomalous c-axis transport properties [5] and to the anomalously large superconducting transition temperatures for these materials [6]. In this theory, both these effects depend on the absence of coherent single-particle tunneling between the layers which is blocked as a result of the "orthogonality catastrophe" being effective as a result of an (assumed) non-Fermi liquid behavior in the planes [4–7]. Also from this point of view it, therefore, seems natural to study the microscopic Josephson coupling between attractive-U Hubbard model planes, which exhibit this non-Fermi liquid characteristic. However, it should also be stressed that the attractive-U model has important short-comings, when compared with the cuprates, especially the absence of the antiferromagnetic order at half-filling and the d-wave symmetry of the superconducting order parameter. This would require a rather extended model, *e.g.* where a next-neighbor attraction and on-site repulsion are included, leading to the appropriate magnetic phase as well as d-wave pairs. In this sense, the present work can be considered as a first step, which aims at clarifying the basics of the microscopic Josephson effect. We believe – and this is confirmed by our numerically essentially exact QMC results – the basics require a short coherence length superconductor in the plane and dynamics perpendicular to the plane, introduced by a vertical hopping.

A simplified mean-field (BCS) description of this model similar to an earlier version by Tanaka [15] is discussed in Section 2. This BCS description is similar in spirit to the conventional Josephson description in that it introduces, in analogy to the standard treatment, the phase dependence of the BCS order parameter (which is constant in a plane) perpendicular to the planes. Despite its limitations, this simple mean-field solution illustrates some of the physics: in particular, the dependence of the supercurrent on the microscopic parameters, *i.e.* the inter-plane hopping and the on-site interaction U. However, it cannot account for the Kosterlitz-Thouless nature of the superconductivity in the planes [8,9,13] and the corresponding power-law pairing correlations.

Section 3 summarizes the QMC evidence for the intrinsic Josephson effect, including a finite-size study with respect to the number of coupled planes (up to 8). The influence of model parameters such as the temperature on the Josephson current is extracted. Of particular interest in view of the above-mentioned "Josephson-pairing" theory [4–6] is that we find at best a mild elevation (for intermediate interaction $U = -4t_p$) of the Josephson transition temperature compared to the 2D Kosterlitz-Thouless temperature. Following an argument of Ferrel [14], this can be understood within a weak-coupling (small U/t_p) BCS framework: in the normal state, single-electron tunneling through the barrier between the two planes lowers the energy of the system. A part of this self-energy is lost when the planes become superconducting because of the gap in the quasiparticle spectrum. The lost self-energy is, however, restored by the tunneling of Cooper pairs and the resulting Josephson coupling energy. In the Strong, Clarke and Anderson scenario the self-energy loss due to single-particle tunneling is assumed to be suppressed and only the energy lowering due to Copper pair tunneling is effective. From the Anderson *et al.* theory point of view our results can be interpreted as demonstrating that the non-Fermi liquid characteristics of the attractive-U Hubbard model are not "robust" enough, to effectively suppress interplane hopping. Finally Section 4 summarizes the results.

2 Description of the model and mean-field evaluation

The superconducting CuO_2 planes in x-y-direction (Fig. 1) are simulated by a 2D Hubbard model with attractive interaction, which is subjected to periodic boundary conditions:

$$H_p = -t_p \sum_{\langle i,j\rangle_\parallel,\sigma} (c^\dagger_{i,\sigma} c_{j,\sigma} + h.c.) - U \sum_i c^\dagger_{i,\uparrow} c_{i,\uparrow} c^\dagger_{i,\downarrow} c_{i,\downarrow} - \mu \sum_{i,\sigma} c^\dagger_{i,\sigma} c_{i,\sigma}. \qquad (1)$$

The summation $\langle i,j\rangle_\parallel$ is taken over nearest neighbors in the planes and t_p, $U > 0$ and μ denote the transfer energy in the plane, the attractive interaction and chemical potential, respectively. The planes are coupled by a hopping term in the perpendicular (z-) direction:

$$H_\perp = -t_z \sum_{\langle i,j\rangle_\perp,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + h.c. \qquad (2)$$

In the z-direction twisted boundary conditions are used. Figure 1 displays the geometry used in the QMC simulations in which the Hubbard planes are stacked into a torus and threaded by a magnetic field. The magnetic field $\mathbf{B}$

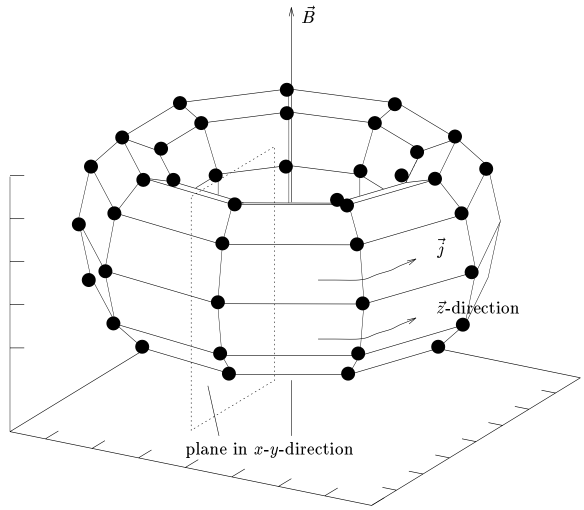

Fig. 1. Schematic view of the used geometry. The coupled superconducting planes are arranged in a torus threaded with a local magnetic field **B**.

in x-direction is confined to the center of the circle. Since the wave function must be single valued, a particle going once around the flux line acquires a phase $\exp\left(\frac{2\pi i\Phi}{\Phi_0}\right)$, where $\Phi_0 = \frac{h}{e}$ is the elementary flux quantum [17] and Φ is the threaded flux. Thus, the fermionic operators are subject to the boundary conditions:

$$c_{\mathbf{i}+N_z\mathbf{e}_z,\sigma} = \exp\left(\frac{2\pi i\Phi}{\Phi_0}\right) c_{\mathbf{i},\sigma} \tag{3}$$

$$c_{\mathbf{i}+N_{x(y)}\mathbf{e}_{x(y)},\sigma} = c_{\mathbf{i},\sigma}. \tag{4}$$

Here $\mathbf{e}_{x,y,z}$ are the lattice vectors of unit length and N_x, N_y, N_z are the linear lengths in the respective directions. Through a canonical transformation, the total Hamiltonian $H = H_p + H_\perp$ may be written as

$$\begin{aligned} H = &-t_p \sum_{\langle i,j\rangle_\parallel,\sigma} (c^\dagger_{i,\sigma}c_{j\sigma} + h.c.) \\ &- t_z \sum_{\langle i,j\rangle_\perp,\sigma} \left(c^\dagger_{i,\sigma}c_{j\sigma}\exp\left(\frac{2\pi i}{N_z}\frac{\Phi}{\Phi_0}\right) + h.c.\right) \\ &- U\sum_i c^\dagger_{i,\uparrow}c_{i,\uparrow}c^\dagger_{i,\downarrow}c_{i,\downarrow} - \mu\sum_{i,\sigma} c^\dagger_{i,\sigma}c_{i,\sigma}. \end{aligned} \tag{5}$$

The fermionic operators now satisfy periodic boundary conditions in both the x- and z-directions. This model can be interpreted as a torus (shown in Fig. 1) built up from stacks of coupled Hubbard x-y-planes and threaded by a **B**-field in the x-direction. As shown in Section 3, this geometrical arrangement is directly accessible to QMC simulations.

The influence of the **B**-field on the Josephson dc-current is described by the gauge-invariant form of the Josephson equation [18,19]:

$$j = \sin\left(\theta_2 - \theta_1 - \frac{2e}{\hbar}\int(\mathbf{A}\cdot \mathrm{d}\mathbf{l})\right). \tag{6}$$

Here $\theta_2 - \theta_1$ denotes the phase difference at zero magnetic field of the two planes considered and $\mathbf{A}$ gives the vector potential induced by $\mathbf{B}$.

In our microscopic model the bare interplane hopping t_z in equation 2 is real (*i.e.* the bare tunneling matrix elements). In this case $\theta_2 - \theta_1 = 0$, and the sinusoidal dependence of the tunneling current stems entirely from the line integral $\int \mathbf{A}\cdot\mathrm{d}\mathbf{l} = \Phi$, *i.e.* the magnetic flux:

$$j = \sin\left(4\pi\frac{\Phi}{\Phi_0}\right)\cdot \tag{7}$$

In order to verify this intrinsic Josephson behavior, the tunneling current perpendicular to the planes (in z-direction, Fig. 1) can be calculated, using the relation [20]

$$\langle \mathbf{j}\rangle = \left\langle\frac{\partial H}{\partial \mathbf{A}}\right\rangle\cdot \tag{8}$$

This current should display a sinusoidal dependence on the penetrating flux $\frac{\Phi}{\Phi_0}$, with period $\frac{1}{2}$.

Let us illustrate the idea by considering first a simplified BCS treatment [15], which is based on a Hartree evaluation of the free energy F and the current

$$j = \left\langle\frac{\partial H}{\partial A}\right\rangle \propto \frac{\partial F}{\partial(\Phi/N_z)}\cdot \tag{9}$$

Here, the interaction part

$$H_{int} = -U\sum_i c^\dagger_{i,\uparrow}c_{i,\uparrow}c^\dagger_{i,\downarrow}c_{i,\downarrow} \tag{10}$$

is simplified to the usual BCS form

$$H_{int} \approx -\sum_i\left(c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}\Delta + h.c. - \frac{|\Delta|^2}{|U|}\right), \tag{11}$$

where $\Delta = |U|\langle c_{i\uparrow}c_{i\downarrow}\rangle$ denotes the pair potential. For an attractive on-site potential, the Cooper pairs have simple s-wave symmetry [9]. The usual phase dependence is introduced by writing the pair potential $\Delta_m = \Delta e^{im\phi}$ for the mth plane.

Fourier-transforming in all spatial directions, this BCS Hamiltonian then can be written:

$$\begin{aligned} H = &\sum_{k\sigma}\epsilon(k)c^\dagger_{k\sigma}c_{k\sigma} - \sum_k \Delta(k)[c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow} + c_{-k\downarrow}c_{k\uparrow}] \\ &+ \sum_k\frac{\Delta^2(k)}{|U|}, \end{aligned} \tag{12}$$

where $k = (k_x, k_y, k_z)$ is the 3D wavevector and

$$\begin{aligned} \epsilon(k) = &-2t_p[\cos(k_x a) + \cos(k_y a)] \\ &- 2t_z\cos\left(k_z a + \left(\frac{2\pi}{N_z}\frac{\Phi}{\Phi_0}\right)\right) \end{aligned} \tag{13}$$

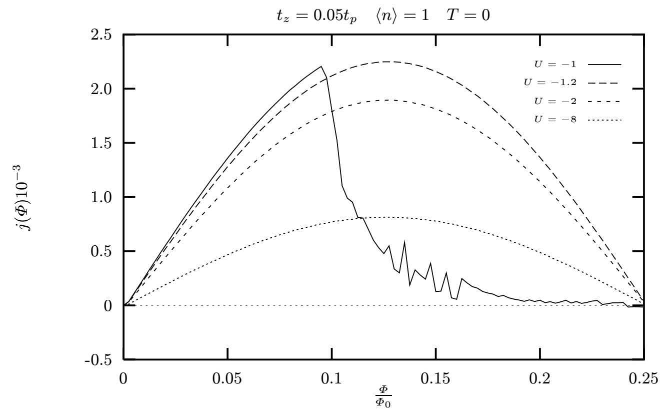

Fig. 2. Mean-Field Current perpendicular to the planes *versus* magnetic flux for $t_z = 0.05t_p$ and various values of U at $\frac{1}{2}$-filling $\langle n\rangle = 1$ and $T = 0\,\mathrm{K}$. The oscillations for $U = -1$ are due to the numerical differentiation.

gives the kinetic energy of the electrons. This Hamiltonian, which is bilinear in its fermionic operators, can be diagonalized using a standard Bogoliubov transformation:

$$H=\sum_k E_k(\alpha^\dagger_{k\uparrow}\alpha_{k\uparrow}+\alpha^\dagger_{k\downarrow}\alpha_{k\downarrow})-\sum_k[\tilde{E}_k-\tilde{\epsilon}_k]+\sum_k\frac{\Delta^2}{U}, \tag{14}$$

where $\tilde{\epsilon}_k = \frac{1}{2}[\epsilon_+(k) + \epsilon_-(k)]$, $\tilde{E}_k = \sqrt{\tilde{\epsilon}_k^2 + \Delta^2}$
and $E_k = \tilde{E}_k + \frac{1}{2}[\epsilon_+(k) - \epsilon_-(k)]$
is the BCS quasiparticle-energy, and

$$\begin{aligned}\epsilon_+(k) &= 2t_p(\cos(k_x a) + \cos(k_y a))\\ &\quad + 2t_z\cos\left(k_z a + \left(\frac{2\pi}{N_z}\frac{\Phi}{\Phi_0}\right)\right) - \mu\\ \epsilon_-(k) &= 2t_p(\cos(k_x a) + \cos(k_y a))\\ &\quad + 2t_z\cos\left(k_z a - \left(\frac{2\pi}{N_z}\frac{\Phi}{\Phi_0}\right)\right) - \mu. \end{aligned} \tag{15}$$

The free energy can be obtained analytically from H, yielding:

$$F=\frac{N\Delta^2}{U}-\sum_k(\tilde{E}_k-\tilde{\epsilon}_k)-2k_BT\sum_k\log(1+e^{-\beta E_k}). \tag{16}$$

The tunneling current $j(\Phi)$ can be obtained by numerically differentiating $F(\Phi)$. The parameter Δ is extracted by minimizing the free energy, resulting in the BCS-type gap equation:

$$\Delta = \frac{U}{N}\sum_k \frac{\Delta}{2\tilde{E}_k}(1 - f(E_k) - f(E_{-k})). \tag{17}$$

A typical result of this simplified analysis is shown in Figure 2, which illustrates the dependence of the mean-field Josephson current on the microscopic parameters, t_z and U (here and in what follows all energies are measured in units of t_p). In Figure 2 the current $j(\Phi/\Phi_0)$ is plotted against the magnetic flux Φ/Φ_0 for $t_z = 0.1t_p$ at half filling and for various values of U. The current shows the expected sinusoidal Φ-dependence with period $\frac{1}{2}$. The maximum current decreases with increasing on-site interaction, because the effective mass of a Cooper pair and thus its localization tendency in a plane scales roughly with U [15]. If the interaction drops below a critical value, the supercurrent vanishes above a critical value of Φ. This behavior can be understood by looking at the energy of the Bogoliubov quasi-particles, which can be written as

$$E_k = \sqrt{\tilde{\epsilon}_k^2 + \Delta^2(k)} - 2t_z\sin(k_z a)\sin\left(\frac{2\pi}{N_z}\frac{\Phi}{\Phi_0}\right). \tag{18}$$

If the pair potential Δ is smaller than the hopping energy t_z, the energy E_k becomes negative for large Φ and, therefore, a quasi-particle is excited, which corresponds to the destruction of a cooper pair. One should notice that for $\Phi = 0$, *i.e.* without an applied **B**-field, E_k is positive for all finite values of Δ, and BCS superconductivity is stable for all finite values of U. Similarly, one can extract the influence of the filling $\langle n\rangle$ on the supercurrent $j(\Phi)$. As expected, $j(\Phi)$ scales with the number of electrons in the system.

What goes wrong in this mean-field approach? In 2D systems, fluctuations drive the critical temperature T_C for the onset of off-diagonal long-range order (ODLRO) down to zero [22]. There exists, however, a Kosterlitz-Thouless transition at a temperature T_{KT}, below which there is quasi-long-range-order (power-law pair correlations) [23]. Due to experimental evidence for intra- and inter-unit-cell Josephson junctions in YBaCuO single crystals [3], it is generally believed that the high-T_C superconductivity is intrinsically 2D in CuO_2 bilayers, coupled together by Josephson currents along the c-axis (our z-axis) direction. There is also clear experimental evidence from the short coherence length (a few lattice parameters) that the 2D superconductivity is different from the conventional BCS one: the typical radius ($\approx$ coherence length) of a Cooper-pair is comparable to the distance between pairs, and in this sense the HTSC are in an intermediate regime between the usual BCS weak-coupling regime and a regime in which pre-existing pairs Bose condense [25,26]. QMC simulations [8,9] have correctly established the short-coherence length Kosterlitz-Thouless type of superconductivity for the 2D attractive Hubbard model. It is therefore natural, to also apply this numerically rigorous QMC procedure to search for numerical evidence for Josephson tunneling in a stack of coupled CuO_2 planes.

We investigate the attractive Hubbard model using the numerically exact Quantum Monte-Carlo (QMC) method for lattices up to roughly $4 \times 4 \times 4$ sites. We wish to emphasize that this approach has the potential to treat this strongly correlated system exactly, thus going far beyond mean-field methods. Furthermore, it provides an approximation-free, numerically exact ansatz, in contrast to most standard analytical techniques, and it yields information about systems much larger than those accessible by exact diagonalization algorithms. In addition, the application of this method to the attractive Hubbard model has the great advantage that the central drawback of fermion QMC calculations, the so-called "sign problem", does not occur. This allows us to perform reliable and stable calculations over a vast parameter range. The main technique is the temperature dependent QMC algorithm in the grand canonical ensemble and its extension to include a flux, which is largely based on the work of reference [10].

3 QMC results

The Josephson current is characterized by the sinusoidal dependence $j(\Phi) = J_0 \sin\left(4\pi\frac{\Phi}{\Phi_0}\right)$. In our actual QMC simulation (see below), we detect also current contributions of the form:

$$j_s(\Phi) = J_s \sin\left(2\pi\frac{\Phi}{\Phi_0}\right),$$

which are due to single-particle tunneling. This is a "finite-size" effect, with $\lim_{N_z\to\infty} J_s = 0$, which has to be separated from the physical effect we are after.

The current

$$\langle \mathbf{j} \rangle = \left\langle \frac{\partial H(\mathbf{A})}{\partial \mathbf{A}} \right\rangle \tag{19}$$

perpendicular to the planes can be calculated using a finite-temperature QMC technique [21] for the geometry of Figure 1. The expectation value in equation (19) can directly be expressed in Green's functions G_{ij}, which are accessible to standard QMC routines, *i.e.*

$$\begin{aligned} j &= -t_z \sum_{\langle i,j\rangle_z \sigma} \left[c^\dagger_{i\sigma} c_{j\sigma} 2\pi i \frac{N_z}{\Phi_0 L} \exp\left(-2\pi i \frac{\Phi}{\Phi_0}\frac{1}{N_z}\right) - h.c.\right] \\ &= -it_z \frac{2\pi}{a\Phi_0}\left[\sum_{\langle i,j\rangle_z,\sigma} c^\dagger_{i\sigma} c_{j\sigma} \exp(-2\pi i \frac{\Phi}{\Phi_0}\frac{1}{N_z}) - h.c.\right], \end{aligned} \tag{20}$$

where $\Phi = A_z L$ with $L = N_z a$ and a is the lattice parameter. Using

$$\langle c^\dagger_{i\sigma} c_{j\sigma}\rangle = \delta_{ij} - \langle c_{j\sigma} c^\dagger_{i\sigma}\rangle = \delta_{ij} - G^\sigma_{ji},$$

the current becomes:

$$\begin{aligned} \langle j \rangle = -it_z \frac{2\pi}{a\Phi_0} \sum_{\langle i,j\rangle_z \sigma} &\left[G^\sigma_{ij} \exp\left(2\pi i \frac{\Phi}{\Phi_0}\frac{1}{N_z}\right)\right. \\ &\left. - G^\sigma_{ji} \exp\left(-2\pi i \frac{\Phi}{\Phi_0}\frac{1}{N_z}\right)\right]. \end{aligned} \tag{21}$$

In the first simulation we used a $4 \times 4 \times 4$ lattice with periodic boundary conditions in all three spatial directions. Because of the limited system size, the results display considerable finite-size effects. In order to separate

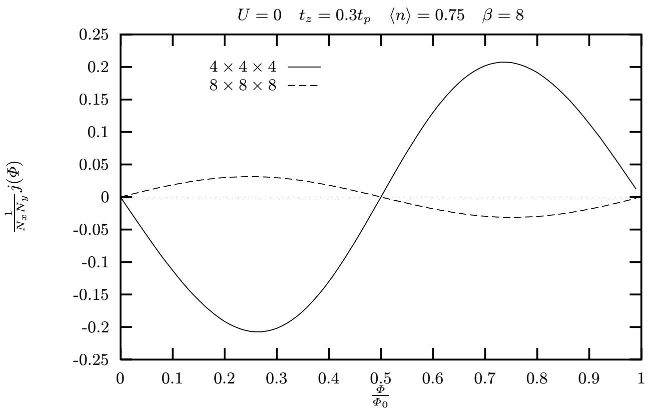

Fig. 3. Current perpendicular to the plane for the non-interacting ($U = 0$) tight-binding model.

these finite-size effects from the physical effect we are after, we have calculated $j(\Phi)$ in the non-interacting ($U = 0$ in Eq. (5)) tight-binding model for two different sizes (Fig. 3). The results show, that the finite-size effects are also sinusoidal, but with period 1, and, indeed (see the argumentation below), they are related to single-particle tunneling. Thus, if a Josephson current appears in the system, $j(\Phi)$ should behave like a superposition of two sinusoidal curves with period $\frac{1}{2}$ and 1. It should, therefore, be of the following additive form

$$j(\Phi) = J_j \sin\left(4\pi\frac{\Phi}{\Phi_0}\right) + J_s \sin\left(2\pi\frac{\Phi}{\Phi_0}\right), \tag{22}$$

with the first term referring to the Josephson supercurrent and the second to the single-particle finite-size effects. The parameters J_j and J_s are the corresponding amplitudes.

The Hubbard model parameters used in the following discussion are: $U = -4t_p$, $\langle n\rangle = 0.75$, $t_z = 0.1t_p$, for which the 2D attractive Hubbard planes are known to show Kosterlitz-Thouless type of superconductivity for $\beta \cong 8$–10 [8,10].

As seen from Figure 4, which contains the QMC results (diamonds plus errorbars), the curve (22) fits the calculated points very well. Thus, we have a first evidence that our model indeed describes a Josephson junction.

By increasing the number of planes from 4 to 8, the amplitude, J_s, of the single-particle finite-size effects can be reduced (Fig. 5), and the sinusoidal curve with period $\frac{1}{2}$ can be seen more clearly. The interpretation of $j_s(\Phi) = J_s \sin\left(2\pi\frac{\Phi}{\Phi_0}\right)$ as a finite-size contribution, that is related to the single-particle tunneling, is based on its scaling behavior as a function of the number of N_z of planes. The reason for this finite-size behavior of j_s can simply be understood: Enhancing the number of coupled planes, N_z, the phase of the single-particle hoppings in equation (5) is more effectively averaged out to zero than for smaller N_z, and J_s should scale to zero.

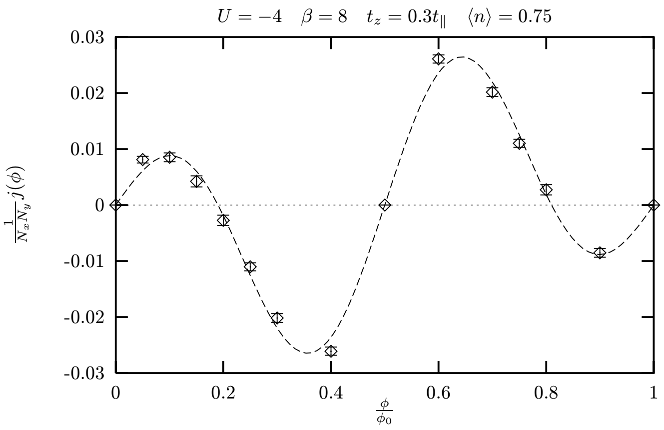

Fig. 4. Current perpendicular to the plane for the 4×4 (planar size) $\times4$ (number of planes) system QMC-results: diamonds plus errorbars, the dotted line shows the interpolated curve $j(\Phi)$.

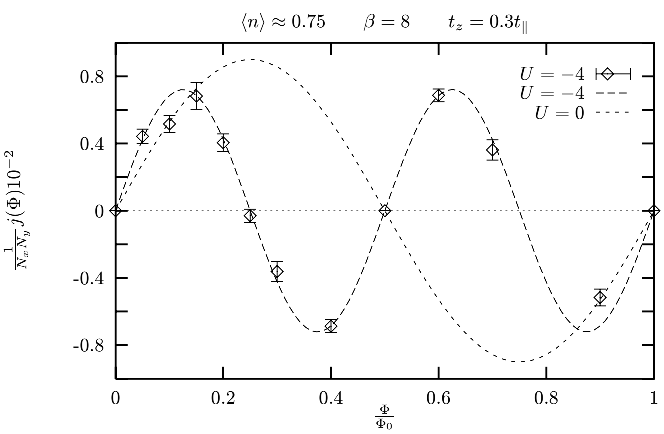

Fig. 5. Current perpendicular to the plane for the $4\times4\times8$ (8 coupled planes in Fig. 1) system. The dashed line shows the $U=0$ behavior.

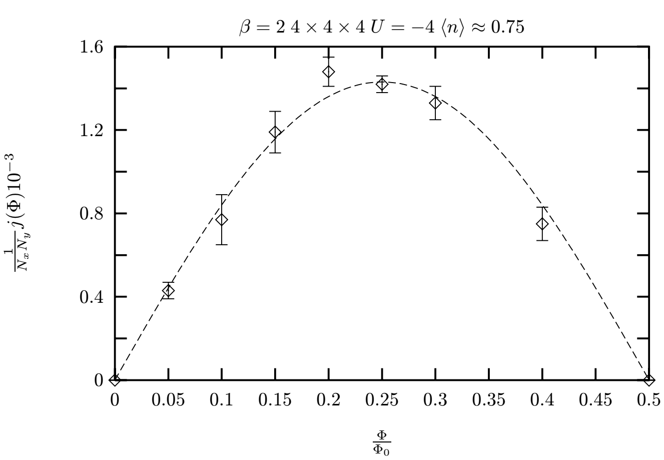

Fig. 6. Current perpendicular to the plane for $\beta t_p=2$.

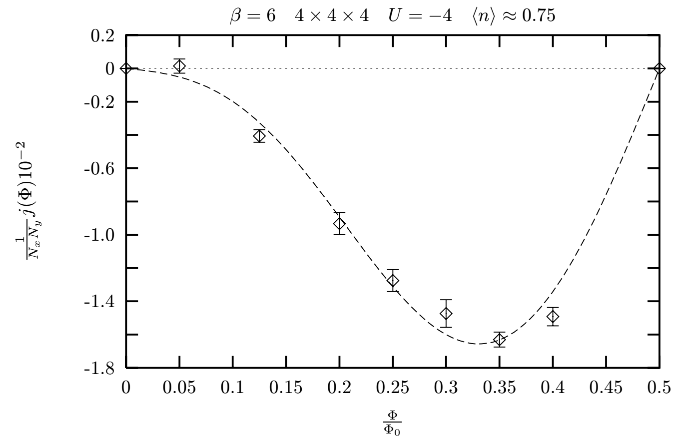

Fig. 7. Current perpendicular to the plane for the same parameters as in Figure 6, however for a three times lower temperature, *i.e.* $\beta t_p=6$.

On the other hand, J_j, the Josephson amplitude, should scale with the number of planes N_z, a relation, which is clearly obeyed by our QMC data in Figures 4 and 5. In Figures 4 and 5, $\dfrac{1}{N_z}j(\Phi)$ is plotted against $\dfrac{\Phi}{\Phi_0}$ for $4\times4\times4$ and $4\times4\times8$ systems, respectively. The lines indicate the interpolated curve. As expected, the magnitudes of $\dfrac{1}{N_z}J_j$ in Figures 4 and 5 are equal ($J_j=0.0079$ is used in both figures). The 2D attractive Hubbard model for $U=-4$ and $\langle n\rangle=0.75$ shows a Kosterlitz-Thouless transition at $\beta_c t_p\approx10$ from the superconducting to a normal phase [9,10]. This transition should be reflected in coupled Hubbard planes, and the Josephson current should break down at some $\beta=\beta_c$. The temperature dependence of j allows an estimation of β_c. In Figures 6, 7 and 8, $j(\Phi)$ is plotted for $\beta=2,6$ and 7 respectively. Figure 4 gives the corresponding plot for $\beta=8$. For $\beta=2$, $j(\Phi)$ is sinusoidal with period 1, *i.e.* no Josephson current appears, and the system is not superconducting. For $\beta=6$ and $\beta=7$, J_j becomes finite, but is still small compared with the value of J_j for $\beta=8$. The J values for $\beta=10$ (not plotted) have been found to be essentially unchanged compared to $\beta=8$. This growing current (with saturation around $\beta\approx8$) is due to interlayer tunneling of local pairing of electrons. For temperatures $\beta\leq8$, exponential not power-law pairing correlations are present in the 2D Hubbard model. Accordingly, preliminary results indicate that for $\beta<8$ the current does not scale with the number of sites in a plane. A rough estimate for the Josephson transition temperature is, therefore, $\beta\cong8$, at best a mild elevation compared to the single plane. Within BCS Ferrel showed that the shift in ground-state energy due to tunneling is the same in the normal and superconducting stats [14]. The physical significance of this result is that the ground-state energy of the junctions in its superconducting state is neither favored nor disfavored, relative to the normal-state energy by the presence of the tunneling barrier. Therefore, in this BCS limit, we do not expect any elevation in the transition temperature.

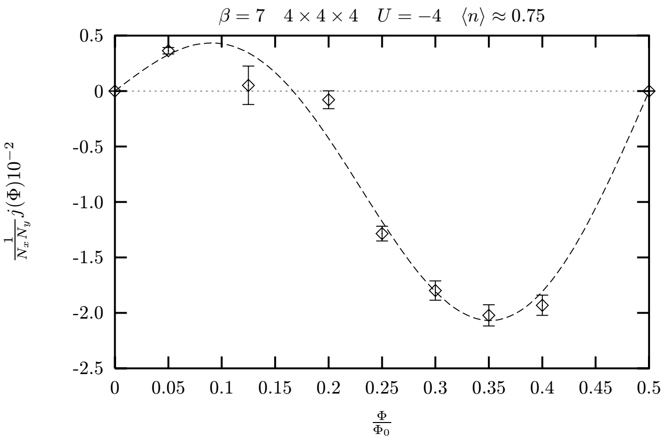

Fig. 8. Current perpendicular to the plane for $\beta t_p = 7$.

4 Conclusions

In this paper, we have presented a model for intrinsic Josephson couplings on a microscopic length-scale. It is based on coupled Hubbard planes with attractive interactions, which are threaded by a local magnetic field. The field dependence of the current $j(\Phi)$ perpendicular to the planes is calculated using numerically rigorous Quantum Monte-Carlo simulations. To extract some of the physical ideas, in particular the dependence on the microscopic parameters U/t_p and t_z/t_p, we first reviewed the mean-field BCS approximation. The maximum current j_{max} increases with decreasing on-site interaction U and increasing hopping energy t_z. At small values of U, for which the pair potential Δ is smaller than t_z, the superconductivity is unstable for finite values of the magnetic flux Φ. In mean-field, the Hubbard model reduces to an effective BCS type Hamiltonian, which is not capable of correctly describing salient features of the 2D superconductivity (short coherence length, Kosterlitz-Thouless transition) in the CuO_2 planes of the HTSC's.

To overcome these shortcomings and to present a rigorous proof of the intrinsic Josephson couplings, we have extracted $j(\Phi)$ from the, in principle (apart from controlled statistical error [21]), exact Quantum Monte-Carlo simulations. The results show a sinusoidal behavior of $j(\Phi)$. A careful discussion of the finite-size scaling of the current clearly reveals that it is the behavior of a Josephson supercurrent. The Josephson current drops to zero for $\beta < 6$, at $U = -4$ and a filling $\langle n\rangle = 0.75$. Due to finite-size effects, this transition is smeared out and, therefore, we can only approximatively determine the transition temperature from superconducting to the normal state at $\beta \cong 8$. These facts give clear evidence that the attractive Hubbard model is capable of describing the Josephson effect in HTSC's on microscopic length scale. Careful studies of the parameter dependence of the maximum supercurrent are under way. These studies should enable us to systematically extract the influence of material properties on the Josephson current, and thus should be useful to optimize the intrinsic Josephson effect for specific applications.

The authors would like to thank D.J. Scalapino and T. Hagenaars for many valueable discussions. One of us (W. Hanke) gratefully acknowledges the hospitality of the Physics Department of the University of California Santa Barbara, where some of this work was carried out. This work was supported by the Bavarian program FORSUPRA.

References

1. R. Kleiner, F. Steinmeyer, G. Kunkel, P. Müller, Phys. Rev. Lett. **68**, 2394 (1992).
2. R. Kleiner, P. Müller, Phys. Rev. B **49**, 1327 (1994).
3. D.C. Ling, G. Yong, J.T. Chen, L.E. Wenger, Phys. Rev. Lett. **75**, 2011 (1995).
4. For recent discussions see P.W. Anderson, Science **279**, 1196 (1998); A.J. Leggett, *ibid*, p. 1157 and K.A. Moler *et al.*, *ibid.*, p. 1193. A.J. Leggett, on the basis of K.A. Moler's experiments, conjectures that materials such as $La_{2-x}Sr_xCuO_4$ and $HgBa_2CuO_{4+\delta}$ can convincingly be argued to follow essential predictions (about the penetration length λ_c) of the interlayer-tunneling, whereas $Tl_2Ba_2CuO_{6+\delta}$ contradicts its predictions by a large margin.
5. D.G. Clarke, S.P. Strong, P.W. Anderson, Phys. Rev. Lett. **72**, 3218 (1994).
6. S. Chakravarty, A. Sudbo, P.W. Anderson, S. Strong, Science **261**, 337 (1993)
7. M. Randeria *et al.*, Phys. Rev. Lett. **75**, 312 (1995).
8. A. Moreo, D.J. Scalapino, S.R. White, Phys. Rev. B **45**, 7544 (1992).
9. M. Randeria, N. Trivedi, A. Moreo, R.T. Scalettar, Phys. Rev. Lett. **69**, 2001 (1992).
10. F.F. Assaad, W. Hanke, D.J. Scalapino, Phys. Rev. B **50**, 12835 (1994).
11. R. Kleiner *et al.*, Phys. Rev. B **50**, 3942 (1994).
12. R. Kleiner, Phys. Rev. B **50**, 6919 (1994).
13. M.Y. Kagan *et al.*, Phys. Rev. B **57**, 5995 (1998).
14. R.A. Ferrel, Phys. Rev. B **38**, 4984 (1988).
15. Y. Tanaka, Physica C **219**, 213 (1994).
16. F.F. Assaad, W. Hanke, D.J. Scalapino, Phys. Rev. Lett. **71**, 1915 (1993).
17. L.H. Ryder, *Quantum Field Theory* (Cambridge University Press, 1985).
18. P.W. Anderson, J.M. Rowell, Phys. Rev. Lett. **10**, 230 (1963).
19. G.D. Mahan, *Many-Particle Physics* (Plenum Press, 1993).
20. J. Wagner, W. Hanke, D.J. Scalapino, Phys. Rev. B **43**, 10517 (1991).
21. E.Y. Loh, J.E. Gubernatis, in *Electronic Phase Transitions*, edited by W. Hanke, Y. Kopaev (Elsevier, New York 1990).
22. S. Schmitt-Rink, C.H. Varma, A.E. Ruckenstein, Phys. Rev. Lett. **63**, 445 (1989).
23. J.M. Kosterlitz, D.J. Thouless, J. Phys. C. **6**, 1181 (1973).
24. J.J. Vicente Alvarez, C.A. Balseiro, Phys. Rev. B **46**, 11787 (1992).
25. A. Tokumitu *et al.*, J. Phys. Soc. Jpn **60**, 380 (1991).
26. M. Drechsler, W. Zwerger, Ann. Phys. **1**, 15 (1992).