Anharmonic Phonons and Electronic Correlations in High-Tc Superconductors : a Quantum Monte Carlo Study

M.Frick[a,b] [1], W.von der Linden[c] and I.Morgenstern[d]

[a] *Institute for Theoretical Physics, University of Groningen, NL-9700 AV Groningen*

[b] *HLRZ, c/o KfA Jülich, D-5170 Jülich*

[c] *Max-Planck Institute for Plasma Physics, D-8046 Garching*

[d] *Institute for Theoretical Physics, University of Regensburg, D-8400 Regensburg*

Abstract. We study a model for high-T_c superconductors describing both the strong correlations and the coupling of the CuO_2-plane carriers to local anharmonic phononic degrees of freedom. Quantum Monte Carlo (QMC) calculations have been performed to investigate ground state properties. The model exhibits superconductivity as characterized by the occurrence of off-diagonal long range order (ODLRO). Several features of the high-T_c materials can be understood. The present calculations have implications in the context of electron-phonon coupling in correlated electron systems in general.

Introduction

Concentrating on the interplay of electron-phonon coupling and electronic correlations in the high-T_c materials, we study the electron-phonon model [1]

$$H = -t \sum_{\langle jj'\rangle\sigma} (c^\dagger_{j\sigma} c_{j'\sigma} + \text{h.c.}) + U \sum_j n_{j\uparrow} n_{j\downarrow} + g \sum_i (\sum_{\delta\sigma} n_{i+\delta\sigma}) s^z_i - \sum_i (\Omega_x s^x_i + \Omega_z s^z_i). \quad (1)$$

$c_{j\sigma}$ describe the carriers with predominant oxygen character (centered around oxygen site j), which form a quasi-particle band upon doping, the Pauli spin matrices s^α_i local external modes centered around Cu site i. These Two-Level Systems (TLS) can represent local anharmonic phononic [2] as well as excitonic modes. Due to correlation effects, the hopping matrix element t reduces to the same order of magnitude as the TLS parameters g, Ω_x, Ω_z, intrigueing a standard Migdal-Eliashberg treatment of (1). We performed Projector QMC calculations [3] to obtain ground state properties.

ODLRO and Superconductivity

Superconductivity is characterized in terms of the occurrence of ODLRO in the two-particle density matrix [4] (also Cooper pair correlation function),

$$\chi_{mn}(l) = \langle c^\dagger_{i+\frac{m}{2}\uparrow} c^\dagger_{i-\frac{m}{2}\downarrow} c_{i+l-\frac{n}{2}\downarrow} c_{i+l+\frac{n}{2}\uparrow} \rangle \to C_{mn} \text{ for } l \to \infty. \quad (2)$$

Instead of solely using the sign of the vertex contribution to χ_{mn} [5], we concentrate on explicite ODLRO [6] to study superconductivity. The condensate is characterized by the Eigenstate corresponding to the largest Eigenvalue of the matrix C_{mn} [4]. The numerical simulations were performed for a two-dimensional lattice. An occurrence of ODLRO is not in conflict with the Hohenberg theorem [7] as the latter only applies to the thermodynamic ensemble at temperature $T > 0$.

[1] Part of the work has been financed by the stichting FOM, which is supported by the NWO.

Results

Fig.1 shows the existence of ODLRO in χ_{11} for a realistic parameter set. After a short distance decay, the pair correlations level off at a non-zero value. Thus, the model exhibits superconductivity instead of the presence of a strong on-site Coulomb repulsion. An investigation of the momentum distribution function [3] favors a BCS picture over the bipolaron szenario. The comparable energy scale of electrons and TLS causes a reduced isotope effect and a short coherence length. The latter can be estimated from fig.2, where the inner structure of the Cooper pair is depicted, as 3-4 lattice spacings. The Coulomb repulsion has rather marginal effects on normal state properties due to the low carrier density. However, the formation of the condensate is dramatically influenced by the repulsion. It poses non-trivial lower bounds on the coupling strength g to the TLS for superconductivity to occur. The presented results have been obtained in a parameter regime that poses severe difficulties on a Migdal-Eliashberg treatment. It is a tempting task to compare the PQMC data with analytical results to find the limit of applicability of both methods in electron-phonon systems.

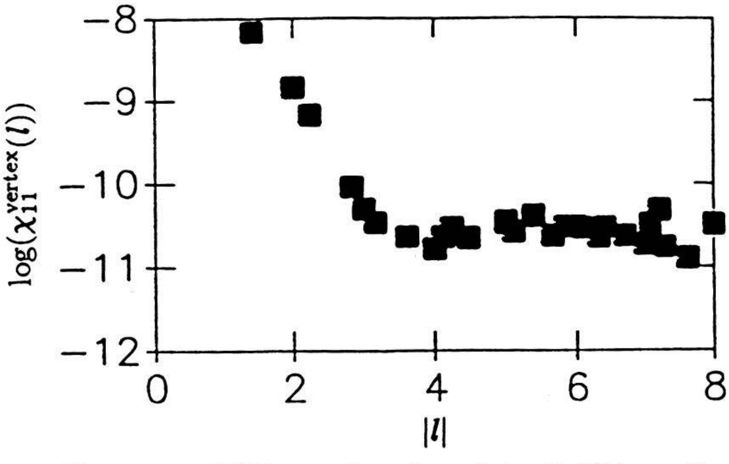

Figure 1. $\chi_{11}^{\text{vertex}}$ as a function of the Euklidean distance $|l|$. $16 \star 16$ lattice, $t = 1$, $U = 6$, $g = 1$, $\Omega_x = \Omega_z = 0.5$, 18 fermions.

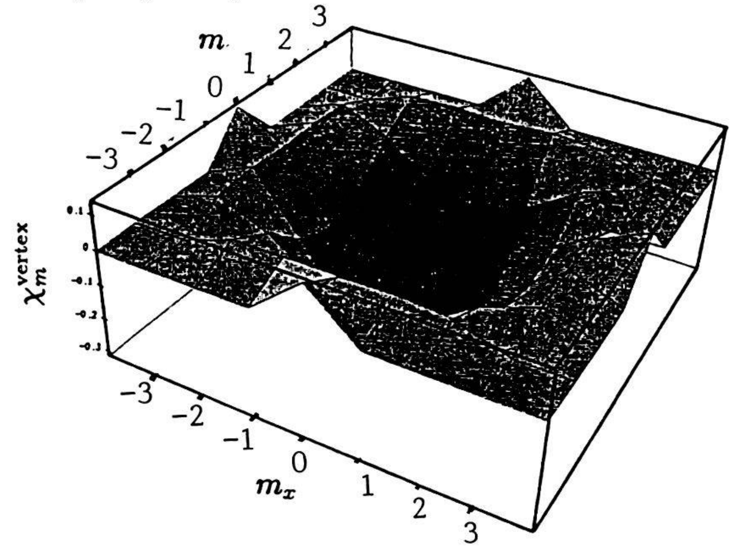

Figure 2. Eigenvector χ_m^{vertex} for the largest Eigenvalue of C_{mn} as a function of the 2D separation $m = (m_x, m_y)$ of the paired electrons. $8 \star 8$ lattice, 10 fermions, parameters see fig.1.

References

[1] M.Frick, I.Morgenstern and W.von der Linden, *Z.Phys.B* 82, 339 (1991)

[2] K.A.Müller, *Z.Phys.B* 80, 193 (1990)

[3] M.Frick, I.Morgenstern and W.von der Linden, *Intl.Jour.Mod. Phys.C*, to be published (1991)

[4] C.N.Yang, *Rev.Mod.Phys.* 34, 694 (1962)

[5] I.Morgenstern, M.Frick and W.von der Linden, *HLRZ preprint* 91-34 (1991)

[6] S.R.White, D.J.Scalapino, R.L.Sugar, E.Y.Loh, J.E.Gubernatis, and R.T.Scalettar, *Phys.Rev.B* 40 , 506 (1989)

[7] P.C.Hohenberg, *Phys.Rev.* 158, 383 (1967)