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BERRYONIC MATTER IN THE CUPRATES

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Abstract A novel form of Jahn-Teller (JT) effect in the cuprates can be reinterpreted as a conventional JT effect on a lattice with a larger unit cell. There is a triplet of instabilities, parametrized by a pseudospin, consisting of a form of the low-temperature tetragonal phase, a charge density wave phase, and a flux phase (orbital antiferromagnet). On a single 4-Cu plaquette, the problem is of $E \otimes (b_1 + b_2)$ form. For a special choice of parameters, the model supports a dynamic JT effect, but is classically chaotic. The connection of this phase with Berryonic matter is discussed.

For stripe phases in the cuprates, an important question is why the charged stripes are metallic: why do they have a preferred doping $x_0 < 1$ hole per Cu? One attractive possibility is that optimal doping corresponds to fixing the Fermi level at the Van Hove singularity (VHS). Then an electronic instability would gap a large density of states, making the holes nearly incompressible and minimizing the electronic free energy ('Stability from Instability.'). It has been proposed that the dominant electronic instability could be to a charge-density wave (CDW) like state [1, 2, 3]. Here I explore the phonon anomalies that might accompany this CDW.

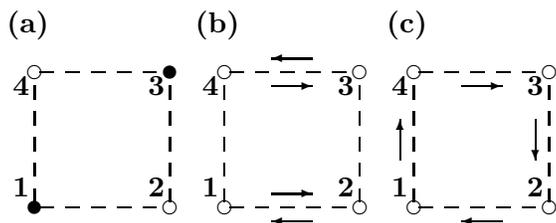


Figure 1. Pseudospin triplet: CDW (a), LTT (b), OAF (c).

There are three related CDW-like distortions which couple to the VHS, all of which have been proposed to play a role in the cuprates. These distortions, which form a pseudospin triplet[4], are illustrated in Fig. 1. The CDW couples to the oxygen breathing mode, which was early proposed as a driving force for high T_c [5] (a dynamic instability of the related half-breathing mode is associated with the stripes[6]). The LTT distortion couples to the strain associated with the low-temperature tetragonal (LTT) phase, which is implicated in pinning the stripes[7]. Finally, the orbital antiferromagnet (OAF) is closely related to the flux phase, a candidate in many theories of cuprate physics[8, 9].

Before the role of stripes was understood, a model was proposed of the low temperature orthorhombic (LTO) phase as a dynamic LTT phase, related to a novel Van Hove – Jahn-Teller (VHJT) effect[10, 3], where the two VHS's constitute the electronic degeneracy. A much deeper understanding of both the phonon anomalies and the VHJT effect can be gained by considering the cuprates as a Berryonic solid[11], with the CuO_2 planes composed of a square array of Cu_4O_8 molecules. Each 2×2 plaquette is Jahn-Teller (JT) active, so the VHJT effect on the original lattice is equivalent to a conventional JT effect on the plaquette lattice. Taking one hole per Cu, the electronic states on a plaquette can be symmetrized to yield states of A_{1g} , B_{2g} , and E_u symmetry. For the lattice as a whole, *all states near the VHS's are built up exclusively of E_u states*[10]. These are the states closest to the Fermi level, and doping the isolated plaquette leads to a conventional $E \otimes (b_1 + b_2)$ JT problem [12]. The B_1 mode couples to the LTT, the B_2 to the CDW, and the dynamic JT phase corresponds to the flux phase.

Here, I study one particular question: in JT terms, under what circumstances could the flux (dynamic JT) phase appear in the plaquette? The relevant parts of the Hamiltonian are the phonon and JT terms:

$$H_{ph} = \frac{1}{2M}(P_1^2 + P_2^2 + M^2\omega_1^2Q_1^2 + M^2\omega_2^2Q_2^2), \quad (1)$$

$$H_{JT} = V_1Q_1T_x + V_2Q_2T_y, \quad (2)$$

with bare phonon frequencies ω_i , electron-phonon coupling V_i , and electronic pseudospins T_i representing the E_u states. The JT energy is $E_{JT}^{(i)} = V_i^2/(2\omega_i^2)$. When $E_{JT}^{(1)} \neq E_{JT}^{(2)}$, the ground state is a static JT distortion, corresponding to the state with larger E_{JT} . More interesting is the case when $E_{JT}^{(1)} = E_{JT}^{(2)}$. If in addition $\omega_1 = \omega_2$, the problem reduces exactly to the well known $E \otimes e$ problem, with anomalous Berry phase[13] signifying the dynamic JT ground state.

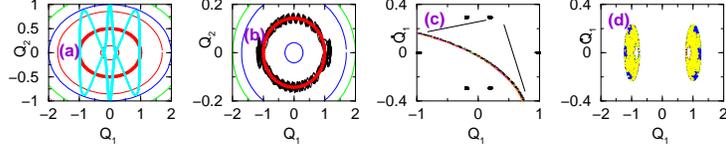


Figure 2. (a,b): Time series, $Q_2(t)$ vs $Q_1(t)$ for $(\omega_2/\omega_1, \beta)$: (a) = (2,1), (b) = (7,0.05394). Ellipses are equipotential contours, with the beaded contour representing the potential minimum. (c,d): Corresponding Poincaré maps. In (c), one attractor is shown on expanded scale.

However, in the cuprates the phonon frequencies ω_1 (LTT) and ω_2 (breathing mode) are very different. Nevertheless, since $V_2 > V_1$, it is possible that $E_{JT}^{(1)} = E_{JT}^{(2)}$ may hold approximately in the cuprates. Curiously, this special case is not well studied. It appears to have a Berry phase (and hence the dynamic JT effect), but is also chaotic. Since the vibronic potential has an elliptic minimum, circulating orbits should be possible, even though the angular momentum j_z is not constant. When the classical Hamiltonian (particle in a non-linear potential well) is numerically integrated, the generic solution is found to be chaotic: the ‘particle’ gets partially trapped near one of the extrema of the ellipse, and after a delay can be reflected or transmitted at random. Some typical trajectories are illustrated in Fig. 2a,b, while the corresponding Poincaré maps (plots of Q_1 vs \dot{Q}_1 when $Q_2 = 0$) are in Figure 2c,d. The data sets are parametrized by $(\omega_2/\omega_1, \beta)$, with β being a scaled initial velocity. For some special initial conditions, nearly periodic solutions can be found, but even for these the Poincaré sections are weakly chaotic. Note that the chaos is present even though the frequencies are rationally related.

The quantum problem has also been analyzed, but so far only in a one-dimensional limit, in which the motion is confined to the bottom of the trough and only ϕ varies. By rescaling the potentials, the potential can be made to have circular symmetry, with anisotropic effective masses. Schroedinger’s equation can be integrated numerically, and it is found that the quantum system shows a ‘memory’ of the classical chaos. Figure 3 shows the time evolution of the most probable ϕ value as a function of time. The wave function remains trapped most of the time in one of the effective potential wells (near the points $Q_2 = 0$), then quickly hops to the next one in a relatively short time. However, the tunneling is coherent, so there is a net circulation. In Fig. 3, results

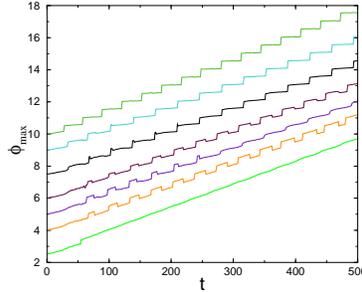


Figure 3. Solution to one-dimensional version of quantum JT problem, showing evolution of ϕ_{max} (the value of ϕ at which the probability density is largest) vs t , for several values of frequency anisotropy: from bottom to top, $\alpha = 0.03, 0.04, 0.06, 0.1, 0.3, 0.6, 1$. Different curves are shifted by assuming different initial positions of the wave function.

for a number of different values of anisotropy $\alpha \equiv (\omega_2^2 - \omega_1^2)/(\omega_2^2 + \omega_1^2)$ are shown. Disregarding some transients, the general trend is that the steps get washed out as the isotropic ($\alpha \rightarrow 0$) limit is approached, but ϕ always contains a monotonic, nearly α -independent component. Hence, in this case also, a flux-phase-like state exists.

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