Quantum Transport in Transition Metal Oxides

Anomalous transport properties in transition metal oxides have been a focus of attention in condensed matter physics since the discovery of high-T_c superconducting materials in cuprates. In these compounds, low-lying excited states are mostly governed by spin degrees of freedom and there are indications to show that the ground state must be a non-Fermi liquid due to strong correlation. Another aspect of the transition-metal oxides, in particular in manganese and ruthenium oxides, is that they are equipped with orbital degrees of freedom; thus, the total internal degrees of freedom consist of both spin and orbital degrees.

In this situation, electronic motion is far from trivial due to complexity of the band dispersion curves even in a simple picture of the band electron; there are numerous crossings and also sensitively affected with spatial arrangements of the internal degrees of freedom, which is very likely to be coupled with lattice distortions through vibronic effects. Even in the cuprate case, the spin band is not simple; on the contrary, one with non-trivial flux is speculated for a certain range of parameters [1].

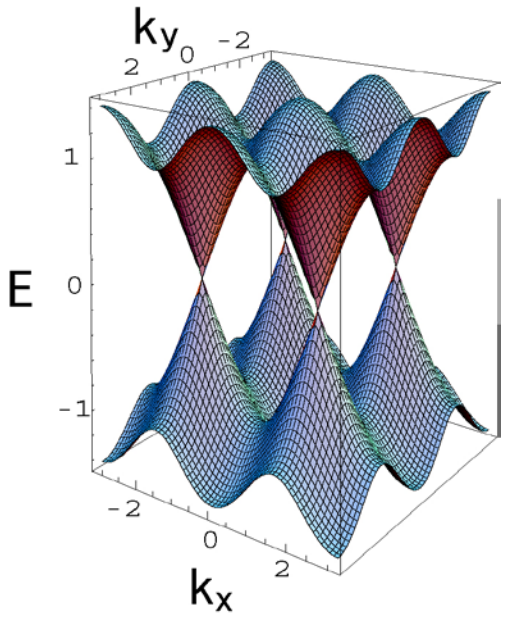

Figure 1: Conically intersecting bands for the flux state in the 2D Hubbard model [1]. The conical intersections are located at $(\pm\pi/2,\pm\pi/2)$. They are the sources of a gauge potential $\mathbf{A}_{n\mathbf{k}}$. Its time-dependence, which may be produced by an adiabatic deformation of the lattice, is predicted to produce a *geometric phase current* in our paper [4].

In order to understand the anomalous current in transition-metal compounds from a viewpoint of the band theory, we have recently reinvestigated the velocity formula for Bloch electrons. Usually the formula is given by $\partial\varepsilon_n(k)/\hbar\partial k$ as is derived in textbooks. In magnetic materials, however, it has been known that it is not valid; instead, a fictitious magnetic field $\mathbf{B}_{n\mathbf{k}}$ has to be included:

$$\frac{1}{\hbar}\frac{\partial\varepsilon_n(\mathbf{k})}{\partial\mathbf{k}} - \dot{\mathbf{k}}\times\mathbf{B}_{n\mathbf{k}};$$

$$\mathbf{B}_{n\mathbf{k}} \equiv \nabla\times\mathbf{A}_{n\mathbf{k}}, \quad \mathbf{A}_{n\mathbf{k}} \equiv i\langle u_{n\mathbf{k}}|\frac{\partial}{\partial\mathbf{k}}|u_{n\mathbf{k}}\rangle,$$

where $\mathbf{A}_{n\mathbf{k}}$ is the gauge potential (*Berry phase connection*) associated with the Bloch electron[2], giving rise to non-trivial geometric phase effects when the crossings of bands exist, or when either time-reversal or inversion symmetry is broken[3].

According to our recent reinvestigation [4], the above formula has to be further modified; an additional term is found in the fundamental expression for the electron velocity. By employing a path-integral representation for the propagator of a Bloch electron, the formula is obtained as

$$\frac{1}{\hbar}\frac{\partial\varepsilon_n(\mathbf{k})}{\partial\mathbf{k}} - \mathbf{E}_{n\mathbf{k}} - \dot{\mathbf{k}}\times\mathbf{B}_{n\mathbf{k}} \quad ; \mathbf{E}_{n\mathbf{k}} \equiv -\frac{\partial\mathbf{A}_{n\mathbf{k}}}{\partial t}.$$

In developing the conventional Fermi-liquid theory, the second and third terms (*Geometric Phase current*) in this velocity formula are not usually taken into account. Thus a further work is called for to elucidate the consequence of these terms, especially in the transition-metal compounds. Note that the second term, which is produced by the fictitious electric field $\mathbf{E}_{n\mathbf{k}}$, explains the adiabatic charge transport processes, which may be relevant in explaining the recently observed anomalous acoustoelectric effect in the film of $La_{0.67}Ca_{0.33}MnO_3$[5].

References

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