Mott insulator

Mott insulators are a class of materials that should conduct electricity under conventional band theories, but are in fact insulators when measured (particularly at low temperatures). This effect is due to electron–electron interactions, which are not considered in conventional band theory.

The bandgap in a Mott insulator exists between bands of like character, such as 3d character, whereas the bandgap in charge transfer insulators exists between anion and cation states,[1] such as between O 2p and Ni 3d bands in NiO.[2]

Contents

History

Although the band theory of solids had been very successful in describing various electrical properties of materials, in 1937 Jan Hendrik de Boer and Evert Johannes Willem Verwey pointed out that a variety of transition metal oxides predicted to be conductors by band theory (because they have an odd number of electrons per unit cell) are insulators.[3] Nevill Mott and Rudolf Peierls then (also in 1937) predicted that this anomaly can be explained by including interactions between electrons.[4]

In 1949, in particular, Mott proposed a model for NiO as an insulator, where conduction is based on the formula[5]

$$(Ni^{2+}O^{2-})_2 \rightarrow Ni^{3+}O^{2-} + Ni^{1+}O^{2-}.$$

In this situation, the formation of an energy gap preventing conduction can be understood as the competition between the Coulomb potential U between 3d electrons and the transfer integral t of 3d electrons between neighboring atoms (the transfer integral is a part of the tight-binding approximation). The total energy gap is then

$$E_{\text{gap}} = U - 2zt,$$

where z is the number of nearest-neighbor atoms.

In general, Mott insulators occur when the repulsive Coulomb potential U is large enough to create an energy gap. One of the simplest theories of Mott insulators is the 1963 Hubbard model. The crossover from a metal to a Mott insulator as U is increased can be predicted within the so-called dynamical mean field theory.

Mottness

Mottism denotes the additional ingredient, aside from antiferromagnetic ordering, which is necessary to fully describe a Mott Insulator. In other words, we might write

antiferromagnetic order + mottism = Mott insulator

Thus, mottism accounts for all of the properties of Mott insulators that cannot be attributed simply to antiferromagnetism.

There are a number of properties of Mott insulators, derived from both experimental and theoretical observations, which cannot be attributed to antiferromagnetic ordering and thus constitute mottism. These properties include

- Spectral weight transfer on the Mott scale [6][7]
- Vanishing of the single particle Green function along a connected surface in momentum space in the first Brillouin zone [8]
- *Two* sign changes of the Hall coefficient as electron doping goes from $n = 0$ to $n = 2$ (band insulators have only one sign change at $n = 1$)
- The presence of a charge $2e$ (with $e < 0$ the charge of an electron) boson at low energies [9][10]
- A pseudogap away from half-filling ($n = 1$) [11]

Applications

Mott insulators are of growing interest in advanced physics research, and are not yet fully understood. They have applications in thin-film magnetic heterostructures and high-temperature superconductivity, for example.[12]

This kind of insulator can become a conductor by changing some parameters, which may be composition, pressure, strain, voltage, or magnetic field. The effect is known as a Mott transition and can be used to build smaller field-effect transistors, switches and memory devices than possible with conventional materials.[13][14][15]

See also

- Hubbard model
- Tight-binding approximation
- Electronic band structure
- Mott criterion
- Dynamical mean field theory
- (Mott) variable-range hopping

Notes

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