Controlling the Mott gap using substrates

Coulomb engineering of Mott insulators

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In Short

- How does substrate screening affect the Coulomb interaction and thereby the Mott gap?
- Use the substrate to engineer desireable properties of monolayer Mott insulators
- Strong correlations and long-ranged interactions

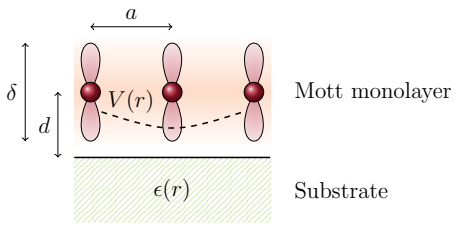

***Figure 1:** Impression of a monolayer Mott insulator on a substrate (not to scale). The Coulomb interaction $V(r)$ between electrons depends on the screening both inside the monolayer and by the substrate. This allows the substrate to be used as a tool to control the properties of the Mott insulator.*

Electrons are responsible for the charge transport in solids. The presence or absence of an energy gap at the Fermi level of the electrons determines if a material is insulating or metallic. Mott insulators are insulators where such a gap is caused by the Coulomb interaction between the (charged) electrons. In a vacuum, the strength of the Coulomb interaction depends only on the distance between the electrons in question. However, the electrons in real materials do not live in a vacuum and the Coulomb interaction is *screened* by other electrons in the material and its surroundings.

We consider a thin layer of a Mott insulating material on top of a substrate, as illustrated in Figure 1. In this case, the Coulomb interaction in the Mott insulator is screened by the substrate. The screening changes the overall magnitude of the Coulomb interaction but it also changes how the interaction depends on the distance. Since the Coulomb interaction is responsible for many electronic properties and in particular for the Mott gap, in this situation the substrate can be used to control these properties of the insulating monolayer: Coulomb engineering.

This scenario is hard to investigate theoretically and computationally. Due to the strong Coulomb interaction, the electrons in Mott insulators are *strongly correlated*. This means that the electrons cannot be treated as independent particles and makes the electronic system difficult to treat computationally. A common approach is to use a simplified model, the Hubbard model, where only the interaction between electrons on the same site is taken into account. That simplified model is already extremely challenging to investigate numerically, but it is also cleary insufficient for this study since the spatial character of the substrate screening is essential.

This requires us to use the dual boson method [1], a modern many-body technique that can deal with strong correlations and with long-ranged Coulomb interactions. With this method, we will determine how the properties of the Mott insulator depend on the substrate. Of particular interest are the electronic density of states and the charge fluctuation spectrum, where the Mott gap is explicitly visible.

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http://www.itp.uni-bremen.de/ag-wehling/

More Information

[1] E. G. C. P. van Loon, A. I. Lichtenstein, M. I. Katsnelson, O. Parcollet, and H. Hafermann, *Phys. Rev. B* **90**, 235135 (2014). doi: 10.1103/PhysRevB.90.235135