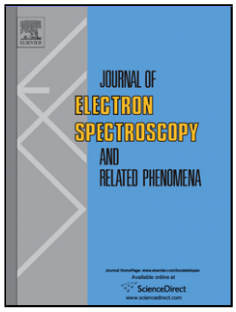

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Single- and many-particle description of scanning tunneling spectroscopy

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Abstract

Scanning tunneling spectroscopy measures how a single electron with definite energy propagates between a sample surface and the tip of a scanning tunneling microscope. In the simplest description, the differential conductance measured is interpreted as the local density of states of the sample at the tip position. This picture, however, is insufficient in some cases, since especially smaller molecules weakly coupled with the substrate tend to have strong Coulomb interactions when an electron is inserted or removed at the molecule. We present theoretical approaches to go from the non-interacting and single-particle picture to the correlated many-body regime. The methodology is used to understand recent experiments on finite armchair graphene nanoribbons and phthalocyanines. We also theoretically discuss the strongly-correlated model system of fractional quantum Hall droplets.

Keywords: Scanning tunneling spectroscopy, Many-body theory, Graphene nanoribbons, Phthalocyanines

1. Introduction

Scanning tunneling spectroscopy (STS) combines atomic spatial resolution with current-voltage spectroscopy, making it possible to probe the electronic structure of single molecules and atoms [1–8]. Such experiments are of fundamental importance for understanding charge and spin transport in nanoscale systems. STS is based on the scanning tunneling microscope (STM), an instrument that measures the quantum-mechanical tunneling current between a conducting sample and a sharp probe tip to generate a topographic image of the sample surface. As will be discussed in detail in this review, the tunneling current depends on the overlap between the tip and sample wave functions, and measurement of the tunneling conductance as a function of applied bias voltage allows deducing the local density of states (LDOS) of the sample.

Measurements on molecular systems are usually interpreted in terms of single-particle molecular orbitals [9–11]. However, while optical spectroscopy probes the excitation spectrum of a molecule with a fixed number of electrons, STS measures the spectrum in case an electron is inserted or removed, due to tunneling between the tip and molecule. If the molecule is small enough, the charging energy to overcome the Coulomb repulsion of the electrons of the neutral molecule can be substantial. Therefore, to describe the eigenstates and -energies of especially the charged molecule properly, it is not clear *a priori* whether the single-particle interpretation suffices. Even so, many-body effects, which have been studied in detail in correlated electron systems such as (high Tc) superconductors [12, 13], are usually neglected. The more general quantity that is applicable beyond the single-particle description, and one that corresponds to LDOS and the STS dI/dV measurements, is the single-particle spectral function [14]. It will be discussed extensively in the current review.

In order to compare to the experimental measurements, one can do theory and calculations in various levels of sophistication. We will discuss mainly the three cases, namely the non-interacting, the single-particle (or mean-field or independent particles), and the interacting many-body picture. The various pictures can be defined by stating that in the first two the states are written as single Slater deter-

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