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80 000 000 000 000 000 000 Atoms

80 000 000 000 000 000 000 atoms are contained in a single grain of sand. Have you ever asked yourself how scientists handle such an inconceivable number of particles without getting dizzy? Well, the answer is simple: Approximations!
But what would be a good approximation to treat so many atoms? One answer would be, by imagining that it is just a single atom instead. This may sound extremely unreasonable, but it turned out that this approximation actually works decently for the type of *strongly correlated materials*.

In the world of Solid State Physics we are interested in creating and improving approximations to determine the electronic properties of materials. With better knowledge of the properties, we can make electric devices faster, more efficient and more precise. Since there are many different types of materials, sadly there is no such thing as one method to approximate them all. Especially the electronic structure of so-called strongly correlated materials often deviate from the truth for traditional approximations.

Strongly correlated materials are called strongly correlated, because the electrons which inhabit the same *orbital* of an atom in the material, experience very strong repulsion from each other. This produces a lot of interesting phenomena like *high-temperature superconductivity*, *colossal magnetoresistance* or *conductor-insulator transitions*. In fact, this repulsion is so strong compared to influences of the electrons from nearby particles, that the *Hubbard I Approximation* gets away by simulating a single atom (or more specifically a single *unit cell*) and mapping the result on the whole solid.

Another interesting phenomenon in solids is the *screening effect* which occurs when an electron leaves the solid. This can be achieved for example by shining light on things. After the electron leaves, a positively charged *hole* is left at its former place instead. Surrounding electrons are then attracted by this *potential* and move closer. These surrounding electrons now screen the hole, so that other electrons feel the presence of the hole much less. This gathering of electrons around the hole is referred to as a quasi-particle. An approximation which incorporates this effect thoroughly, is the so-called *GW Approximation*.

In this thesis work, the Hubbard I Approximation and the GW Approximation were combined to include both strong correlation and screening effects for a one-dimensional model. The inclusion of both these effects were indeed observed in the results. Moreover, since the two methods partially cover the same effects, *double-counting* appears in the combination. Three approaches were tested to mitigate this problem.

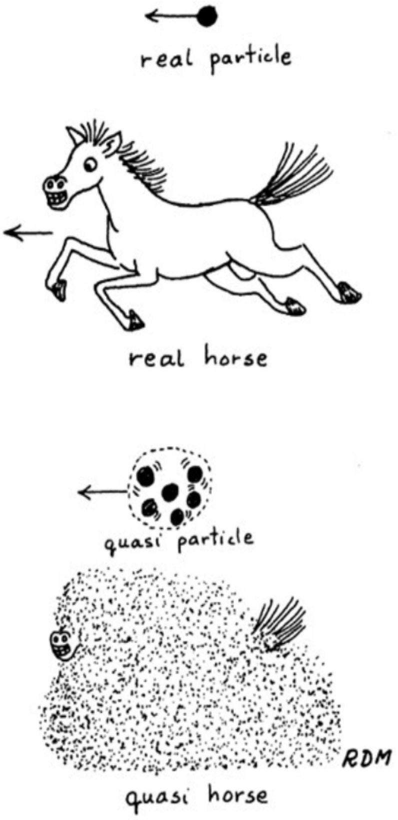

Illustration by Richard D. Mattuck
from “A Guide to Feynman Diagrams
in the Many-Body Problem”

“Combining the GW Approximation with the Hubbard I
Approximation for strongly correlated materials”

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