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Ground-State Properties of the Hydrogen Chain: Dimerization, Insulator-to-Metal Transition, and Magnetic Phases

Sections I–IV.

The text is about 29k symbols.

Vocabulary

retain	сохранять	page 1, abstract
intricate	сложный, запутанный	page 1, abstract
intertwined	переплетенные	page 1, abstract
profoundly	очень, глубоко	page 1, par. 1 (right)
tractability	управляемость	page 2, par. 3 (left)
hallmark	отличительная черта	page 2, par. 3 (left)
synergistic	синергетический	page 2, par. 4 (left)
diffuse	расплывчатый, размытый	page 3, par. 3 (left)
envelope	огибающая	page 3, last par. (left)
illuminating	хорошая иллюстрация	page 3, last par. (right)
bond	связь	page 4, par. 2 (right)
commensurate	соизмеримый, соразмерный	page 5, last par. (left)
cusp	пик, острие	page 6, par. 1 (left)
degeneracy	вырождение	page 6, par. 1 (left)
kink	излом	page 6, par. 1 (right)
instantiate	приводить в пример	page 7, last par. (left)
in silico	путем моделирования	page 7, par. 2 (right)

Questions

1. What system do the authors investigate?
2. How is dimerization first probed in this work?
3. How does it manifest itself apart from the electron density?
4. What type of materials often exhibits metal-insulator transitions?
5. What parameters should be varied if metal-to-insulator transition is to be observed?
6. What is the ground state of a one-band model with commensurate filling?
7. Where does the metal-to-insulator transition arise from in the hydrogen chain?
8. What is responsible for metallic behavior in multi-band systems?
9. What effects are absent in Hubbard model which give rise to the hydrogen chain conductivity?

10. Who pioneered the study of the metal-to-insulator transition?
11. What was the revolutionary approach to constructing electron wave-functions?
12. How can the physics described in the article be realized experimentally?

Overview

Regarding electrical conductivity, here exist three types of materials: insulators, semiconductors, and conductors (also called metals). Of the three of them, the most interesting and complex is of course semiconductors. But the other two kinds are far from being fully understood and described. We know that insulators have electron densities localized in the vicinity of atoms or inside molecules. Considering metals, we know that they form a unique lattice structure of positively charged ions and almost completely free electrons between them that can be even perceived as a gas. For a more comprehensive look at the nature of electrical conductivity, we have to simulate the whole atomic system and derive conditions under which it behaves as a metal or as an insulator. The difficult part here is in calculations. Quantum systems, which atomic materials obviously are, need to satisfy specific symmetries of their wave-function, and the more electrons they contain, the more complex are the bounds and hence the calculations. The complexity grows exponentially with the size of the system. Quantum computing may help us perform such computations more easily, but for now we have to work with smaller systems.

The authors work with a system of N identical hydrogen atoms equidistantly located along the z axis. To further simplify the system, the protons are considered fixed in place, so there are just N electrons moving in a certain potential. The aim was to analyze how the electrons behave for different proton separations and various numbers of atoms. Even with this kind of simplification, regular straightforward methods don't yield any rational results, so the authors used several numerical methods and tried to identify a consistent result.

The authors started from a large separation. In this case, each electron is localized near the corresponding proton, and their energy levels are almost the same as of isolated atoms. However an interesting effect occurs anyway. Although energy levels are almost the same, the electrons, being part of a single quantum system, feel each other by symmetries of the wave-function. So at large separations, when the Coulomb interaction between the electrons is weak, they align their spins in opposite directions. This way, the hydrogen chain exhibits antiferromagnetic correlations which fade a bit faster than a simple approach yields; probably due to the finite size of the chain.

When the protons are brought closer, they start forming pars called dimers. The most obvious consequence of dimerization is that the electron density between a proton and its right neighbor differs from the density between it and the left neighbor. This effect is very

subtle and hard to capture numerically, but three of five fundamentally different methods used by the authors gave approximately the same result for the difference in electron density depending on the length of the hydrogen chain, which is very impressive. More evidence of the dimerization is contained in kinetic energy and entanglement entropy.

For short proton separations, the most interesting effect to study is the metal-to-insulator transition (MIT). According to some of the most successful phenomenological models of three-dimensional conductors, there should be no such transition at all. However, it occurs for two reasons. The first is that single-atom energy levels broaden in presence of other atoms. The closer they are, the wider the levels become. And there comes a point when the highest occupied level overlaps with the lowest vacant level, and electrons don't need much energy to travel the chain. The second reason is a bit more technical. The quasi-wave-vector induced by the periodic structure gains a second allowed value closer to zero caused by self-doing. This allows some electrons diffuse along the chain axis and thus conduct electricity. It should be noted that fewer methods yielded consistent results here, but it's a generally more complex task, so the agreement is satisfactory.