The Hubbard model and optics: reflectivity of 1D and 2D systems

Vladan Celebonovic
Institute of Physics, Univ. of Belgrade, Pregrevica 118, 11080 Zemun-Belgrade, Serbia
E-mail: vladan@ipb.ac.rs

Abstract. The Hubbard model (HM) was proposed around the middle of the last century as a model of the behavior of correlated electrons. It has so far been solved only in the 1D case. The HM is used in condensed matter physics in work on high $T_c$ superconductors, organic conductors, graphene, ... It is known that reflectivity is related to the electrical conductivity, and both quantities can be measured.

This paper is divided into several sections. It begins with a brief introduction to the HM, and the links between the reflectivity and conductivity of a material with its parameters. In the second and third parts, the explicit calculations of the reflectivity of a 1D and 2D square rectangular lattices will be presented. Expressions for the reflectivity thus obtained are tied to the material parameters via previous results of the author on the conductivity of a 1D lattice. We attempt to find a set of material parameters in both cases of lattices, for which the reflectivity becomes close to zero, or equal to an arbitrary constant. If such a set of material parameters could be found, it could have interesting applications in material science such as invisibility.

1. Introduction

1.1. The Hubbard model

The theoretical framework which is now called "The Hubbard model" (HM) is the achievement of the British physicist John Hubbard (1931 – 1980). Despite the fame and wide applicability of his model, only a couple of biographies of Hubbard are easily accessible. One of them is posted at http://theor.jinr.ru/~kuzemsky/hubbio2.html. He was a brilliant scientist and a very discrete person.

Around the middle of the last century, the problem of the metal-insulator (MI) transition was high on the list of open problems of condensed matter physics. A certain amount of success in analyzing the MI transition was achieved in the early days of quantum mechanics ([1] and references given there). A more general theory of MI transitions was formulated towards the middle of the last century [2]. The first microscopic theory of the (MI) transition has been proposed in [3], and this marked the start of the development of the (HM).

At first glance, the HM seems to be extremely simple. The Hamiltonian by which it is defined contains only two terms: the "free" kinetic term $H_0$ and the "interaction" term $H_I$

$$H = H_0 + H_I$$

(1)

Complexity quickly becomes visible when this Hamiltonian is written completely. In two dimensions, using the second quantisation formalism, it has the form:
\[ H = - \sum_{ij} \sum_{\sigma} \sigma \sigma \sum_{ij} t_{ij} c_{i\sigma}^+ c_{j\sigma} + \frac{1}{2} \sum_{ijkl} \sum_{\sigma \sigma'} < ij | v | kl > c_{i\sigma}^+ c_{j\sigma}^+ c_{l\sigma'} c_{k\sigma'} \] (2)

In this expression, latin indices denote sites on a lattice, \( \sigma \) is the spin index, and symbols of the form \( c_{i\sigma}^+ \) denote second quantisation operators creating an electron with spin \( \sigma \) at a lattice site \( i \). The hopping integral between sites \( i \) and \( j \) is denoted by \( t_{ij} \). Finally, \( v \) is the Coulomb potential. Performing any kind of a calculation with such a Hamiltonian would be prohibitively complicated. However, Hubbard introduced two simplifying assumptions which take into account the essential physics and ease the mathematics. They can be expressed as:

\[
t_{ij} = \begin{cases} 
  t \ (i, j) \ nn \\
  0 \ otherwise 
\end{cases}
\]

and

\[
<i j | v | kl > = \begin{cases} 
  U \ (i = j = k = l) \\
  0 \ (otherwise) 
\end{cases}
\]

where \( nn \) denotes nearest neighbors.

In spite of the fact that it was proposed nearly 60 years ago, the HM has so far been solved analytically only in the 1D case [4]. The interest of this model for the condensed matter community can be appreciated by the number of papers which use it in some way. A search at http://prola.aps.org performed at the time of this writing (end of July 2012) with the keyword ”Hubbard model” has given 1981 paper containing those words in the title or abstract published in Phys.Rev.Lett. and Phys.Rev.B in the period 2000 - 2012.

Knowledge of the Hamiltonian of a system opens up the possibility of calculating its transport properties. One of the methods for such calculations is the so called ”memory function” method, developed in the 1970s as a consequence of previous work of Kubo. Within this method, the conductivity is determined by the following equations:

\[
\chi_{AB}(\omega) = << A; B >> = -i \int_0^\infty \exp i \omega t < [A(t), B(0)] > dt
\] (3)

where \( A = B = [j, H] \), \( j \) denotes the current operator, and

\[
\sigma(\omega) = i \omega^2 P \frac{4 \pi^2}{\chi_0} [1 - \frac{\chi_0}{\chi}] 
\] (4)

The symbol \( \omega_P \) denotes the plasma frequency, which is given by \( \omega_P^2 = 4 \pi e^2 n / m \), and where \( e, n, m \) are the electron charge, number density and mass respectvely. The current operator is defined as follows [5]:

\[
j = \frac{\partial}{\partial t} P = i[H, P]
\] (5)

where

\[
P = \sum_i R_i n_i
\] (6)

is the polarisation operator. In expression (6) \( R_i \) denotes the position of lattice site \( i \), and \( n_i \) is the number of particles at lattice site \( i \). Using the 1D Hubbard Hamiltonian and the
so-called memory function method, it was shown that the electrical conductivity of a 1D system of correlated electrons is given by [6]

$$\sigma_R(\omega) = (1/2\chi_0)(\omega_P^2/\pi)[\omega^2 - (bt)^2]^{-1}(Ut/N^2)^2 \times S$$  \hspace{1cm} (7)

and the symbol $S$ denotes the following function

$$S = 42.49916 \times (1 + \exp(\beta(-\mu - 2t)))^{-2} + 78.2557 \times (1 + \exp(\beta(-\mu + 2t\cos(1 + \pi)))^{-2} + (bt/\omega_0 + bt)) \times (4.53316 \times (1 + \exp(\beta(-\mu - 2t)))^{-2} + 24.6448(1 + \exp(\beta(-\mu + 2t\cos(1 + \pi)))^{-2})$$  \hspace{1cm} (8)

where $b = -4 \times [1 + \cos(1 - \pi)] = -1.83879$, $\mu$ denotes the chemical potential of the electron gas on a 1D lattice determined in [6], $N$ is the number of lattice sites. The immaginary part of the conductivity is given by

$$\sigma_I = \frac{\omega_P^2}{4\pi\omega} \left(1 - \frac{\chi_R}{\chi_0}\right)$$  \hspace{1cm} (9)

and

$$\chi_R(\omega) \equiv \frac{[128U^2t^4\cos^2((1 - 2\pi)/2)][1 + \exp(\beta(-\mu - 2t))]^2N^4(\omega + 2bt)^2]}{[1 + \exp(\beta(-\mu - 2t))]^2}$$  \hspace{1cm} (10)

1.2. Relation with optics

According to standard optics [8] the propagation of an electromagnetic signal through a medium is defined by the frequency dependent dielectric function $\epsilon(\omega)$ and the refractive index $N(\omega) = [\epsilon(\omega)]^{1/2}$. Both can be expressed as complex functions:

$$\epsilon(\omega) = \epsilon_R(\omega) + i\epsilon_I(\omega)$$  \hspace{1cm} (11)

and

$$N(\omega) = n(\omega) + iK(\omega)$$  \hspace{1cm} (12)

where $K(\omega)$ is the extinction coefficient. The real and imaginary components of the dielectric function can be expressed as

$$\epsilon_R(\omega) = n^2 - K^2$$

$$\epsilon_I(\omega) = 2nK$$  \hspace{1cm} (13)

The dielectric function $\epsilon(\omega)$ is related to the susceptibility $\chi(\omega)$ by: $\epsilon = 1 + 4\pi\chi$ and the reflectivity $R(\omega)$ is defined as the ratio

$$R(\omega) = \frac{(n - 1)^2 + K^2}{(n + 1)^2 + K^2}$$  \hspace{1cm} (14)

Our aim is to introduce various material parameters into this definition: the only way to achieve it is to use the electrical conductivity, which is itself a function of material parameters.
The conductivity can be expressed as a complex function, and it is related to the dielectric function by

\[ \epsilon_R(\omega) + i\epsilon_I(\omega) = 1 + i\frac{4\pi(\sigma_R(\omega) + i\sigma_I(\omega))}{\omega} \] (15)

Using expressions for the real and imaginary parts of \( \epsilon \) and \( \sigma \), some algebra leads to

\[ n = \frac{2\pi\sigma_R}{\omega K} \] (16)

and

\[ K^4 + K^2(1 - \frac{4\pi\sigma_I}{\omega}) - \left(\frac{2\pi\sigma_R}{\omega}\right)^2 = 0 \] (17)

Solving for \( K \) gives

\[ K_{1,2}^2 = \frac{4\pi\omega\sigma_I - \omega^2 \pm [(4\pi\omega\sigma_R)^2 + (\omega^2 - 4\pi\omega\sigma_I)^2]^{1/2}}{2\omega^2} \] (18)

Inserting results for \( n \) and \( K \) into eq.(10) leads to the final expression for the reflectivity

\[ R = \frac{(2\pi\sigma_R)^2 - K\omega[4\pi\sigma_R - K\omega(1 + K^2)]}{(2\pi\sigma_R)^2 + K\omega[4\pi\sigma_R + K\omega(1 + K^2)]} \] (19)

Using the fact that \( (1 - ax)/(1 + ay) = (1 - ax) \sum_{l=0}^{\infty}(-1)^l(ay)^l \) (19) can be transformed into

\[ R \approx 1 - \frac{2K\omega}{\pi\sigma_R} + 2\frac{(K\omega)^2}{(2\pi\sigma_R)^2} - \frac{3}{2}\frac{K\omega}{\pi\sigma_R}^3 + \ldots \] (20)

This result is valid regardless of the dimensionality of the system under study. The remainder of this contribution is devoted to the calculation of the function \( R \) for 1D and 2D systems, using results obtained through the HM.

2. Reflectivity of a 1D lattice

Imagine, as a first example, that the aim is to calculate the reflectivity of a 1D nonconducting lattice. This means that \( \sigma_R \to 0 \). Calculating the ratio \( K/\sigma_R \) for this case, it can be shown that \( K/\sigma_R \to \infty \), and this means that \( R \) becomes unphysically large. The implication is that this calculation cannot be applied to insulators.

However, if the conductivity of a 1D lattice is finite, the situation becomes more interesting. Assuming that the number of lattice sites \( N \) and the frequency \( \omega \) are sufficiently large, eqs.(9) and (10) show that the imaginary part of the conductivity \( \sigma_I \to 0 \). Taking the square root of eq.(18) and inserting the result into eq.(20), one gets the following expression for the reflectivity of a 1D lattice

\[ R \approx 1 - \frac{\omega^2}{\pi^2\sigma_R^4} + \frac{[\omega^4 + 16\pi^2\sigma_R^2\omega^2]^{1/2}}{\pi^2\sigma_R^2} \ldots \] (21)

In order to obtain theoretical data meaningfully comparable with experiments, the first step is to obtain values of the conductivity. As an example, figure 1 represents the dependence of \( \sigma_R \) on the temperature \( T \) calculated by eqs.(7) and (8) for the following set of HM parameters: \( N = 150, U = 4t, \omega_p = 3U, \omega = 0.7U, s = 1, n = 0.8, b = -1.83879 \), where various symbols denote: \( N \) is the number of lattice sites, \( s \) is the value of the lattice constant, \( U \) is the Hubbard U, \( t \) is the hopping energy, \( \omega_p \) is the plasma frequency, \( \omega \) denotes the frequency. The conductivity is normalized to \( \sigma_R = 1 \) for \( t = 0.005, T = 116K \) [6].
Knowing the function $\sigma_R(T)$, the next step in the calculation is to determine the function $R(T)$. This can be done by inserting the values of the normalized conductivity into the expression for $R$. For values of the conductivity shown on figure 1, one gets the representation of the curve $R(T)$ shown on figure 2.

Similar curves could be obtained for other choices of the parameters.

3. Reflectivity of a 2D lattice

A more complicated, but also more interesting system, is the rectangular Hubbard plane: a 2D rectangular plane made up of two 1D lattices intersecting at right angles at mutual distance $a$. The reflectivity of a Hubbard plane can be calculated by starting from the 2D Hubbard Hamiltonian, calculating the electrical conductivity and then the reflectivity. A simpler way to perform this calculation would be to define the conductivity of the lattice as $\sigma_r \to \sqrt{\sigma_{rx}^2 + \sigma_{ry}^2}$ as in [7], where the suffixes denote the two coordinate axes, and then determine the reflectivity. It is assumed in this definition that the conductivities along the two lattice axes are mutually independent.

Introducing this definition into eq. (20) for the reflectivity, it follows that

$$R \approx 1 - \frac{2K\omega}{\pi \sqrt{\sigma_{rx}^2 + \sigma_{ry}^2}} + 2\left(\frac{\omega K}{\pi \sqrt{\sigma_{rx}^2 + \sigma_{ry}^2}}\right)^2 - \frac{3}{2}\left(\frac{K\omega}{\pi \sqrt{\sigma_{rx}^2 + \sigma_{ry}^2}}\right)^3 + ...$$  \hspace{1cm} (22)
In the two dimensional case the function $K$ can be defined using the same reasoning for both the real and imaginary components of the conductivity. Taking that $\sigma_{tx} = \sigma_{ty} = 0$ and introducing $\alpha = \sigma_{ry}/\sigma_{rx}$, it follows that

$$K^2_{1,2} = -\frac{1}{2} \pm \frac{1}{2\omega^2}[(4\pi\omega\sigma_x^2 \sqrt{1 + \alpha^2})^2 + \omega^4]^{1/2}$$

(23)

These two expressions open up the possibility of investigating the reflectivity as a function of various material parameters defined within the HM, but also on the ratio of the conductivities along the lattice axes. It follows from eq.(23) that

$$\frac{K\omega}{\pi\sqrt{\sigma_x^2 + \sigma_y^2}} = \frac{K\omega}{\pi\sigma_x \sqrt{1 + \alpha^2}} = \frac{\omega}{\pi\sigma_x \sqrt{1 + \alpha^2}} \left[-\frac{1}{2} + \left(\frac{1}{2\omega^2}\right)[16\pi^2 \omega^2 \sigma_x^4 (1 + \alpha^2) + \omega^4]^{1/2}\right]^{1/2}$$

(24)

Take as an example that $\alpha = 0$, which means that the lattice is not conducting in the $y$ direction. In this case, the conductivity and reflectivity of a 2D plane are given by the expressions for a 1D system. Take as a next example that $\alpha = 0.1$. This means that the conductivity in the $x$ direction is 10 times higher than the value along the $y$ axis. Such a material would be highly anisotropic, and its reflectivity would depend on the temperature in the following way:

Assuming that $\sigma_{ry} = 0.5\sigma_{rx} = \sigma$, that is $\alpha = 1/2$, it follows that

$$\frac{K\omega}{\pi[\sigma_{rx}^2 + \sigma_{ry}^2]^{1/2}} = \frac{2\omega}{\pi\sigma \sqrt{3}} \left[-\frac{1}{2} + \frac{1}{2\omega^2}[\omega^4 + 20\pi^2 \omega^2 \sigma^4]^{1/2}\right]^{1/2}$$

(25)
and the reflectivity follows by inserting this result into eq. (22).

An example of the temperature dependence of the reflectivity of a Hubbard plane is shown in figure 4. The points were calculated for the same values of the $HM$ parameters as used for figure 1, and it was assumed that the ratio of conductivities along the two axes is 1/2. The results were normalized to $R = 1$ at the point $t = 0.005 \beta = 116$.

Figure 3. normalized reflectivity of a 2D lattice, for $\sigma_{ry} = 0.1 \sigma_{rx}$
Another example is shown in figure 5. All the parameters were kept the same, except the ratio of the conductivities, which was increased to \( \alpha = 1 \).

4. Discussion and conclusions

In this paper we have discussed a seemingly purely theoretical subject - the calculation of reflectivity of 1D and 2D systems described by the HM. The obvious question is whether our calculation has any link with real material science, or it is just an interesting problem in mathematical physics. The links exist and are important. In general terms, standard electrodynamics shows that electrical conductivity of many physical systems is related to their reflectivity [8]. A logical consequence is that measuring, or calculating, one of these quantities, one can gain information about the other. The 1D calculation discussed in the present paper has applications in research on highy anisotropic materials.

Examples of such materials are the so-called Bechgaard salts, whose generic chemical formula is \((TMTSF)_2X\) or transition metal oxides, such as \(Tl_2Ru_2O_7\) [9]. Here \(TMTSF\) denotes a highly complicated molecule called tetra-meta-thio-seleno-fulvalene, and \(X\) is some anion. These materials are characterized by a high degree of anisotropy: the ratio of electrical conductivities along the three crystal axes is typically \(\sigma_x : \sigma_y : \sigma_z \cong 1 : 0.01 : 0.001\), which implies that they can be modelled as effectively one dimensional. For recent reviews of some aspects of research on \((TMTSF)_2X\) see, for example [10], [11].

As a simple extension of the calculation for 1D, we have performed the calculation of reflectivity for a 2D rectangular lattice. Purely mathematically, the main point which made

**Figure 4.** normalized reflectivity of a 2D lattice, for \(\sigma_{ry} = 0.5\sigma_{rx}\)
Figure 5. normalized reflectivity of a 2D lattice, for \( \sigma_{xy} = \sigma_{xx} \)

this calculation possible was defining the conductivity of this lattice as \( \sigma = \sqrt{\sigma_x^2 + \sigma_y^2} \), where \( x, y \) denote the two lattice axes. Previous work [6] has shown that the conductivity of a 1D lattice is a function of tunable constants and the temperature to which the specimen is subdued. In the 2D case, one more parameter has to be added - the ratio of conductivities along the two axes, which is a pure number, denoted here by \( \alpha \), characterizing the isotropy of the lattice. No attempt was made to obtain an analytical expression for the reflectivity of a 2D lattice. Instead of such an attempt, the conductivity was calculated for a 1D case with the same choice of parameters as in [6], and this result was then applied to the two dimensional case for several values of the ratio of the conductivities along the two axes.

The results are shown on the figures. With all the other parameters kept constant, the reflectivity at sufficiently low temperatures is influenced by the ratio of conductivities along the lattice axes. For the same value of the temperature, the reflectivity is higher for \( \alpha = 1 \), than for \( \alpha = 0.5 \). This result should be checked for several more values of \( \alpha \).

The 2D part of calculations reported here can find applications in work on conducting materials with 2D structure. It may seem from the figures that the behavior of the reflectivity for 1D and 2D lattices is strikingly similar. This is due to the definition of the conductivity of a 2D lattice which was used. However, the factor which regulates the form of the temperature dependence of the reflectivity of a 2D lattice is the ratio of conductivities along the two lattice axes.

A 2D material in which there is enormous interest at present is of course graphene. However, our results cannot be directly applied to graphene, because it has a honeycomb lattice. On the other hand, it is known that graphene has negligible reflectivity [12]; note figure 3 at \( T \approx 60K \). Another 2D material with considerable biomedical interest is human skin. Calculating, and even more so measuring its reflectivity could be of high interest in surgery, for example in cases of
burning.

Lowering the value of reflectivity of an object, naturally brings into mind the topic of invisibility. Non-radiating objects are visible because they reflect incident light. Objects which do not reflect light, can not be seen - they are invisible. Numerous publications have appeared on the problem of achieving invisibility of various objects by embedding them in different kinds of cloaks (for example [13]). Equations for the reflectivity which we have obtained express it as a function of various material parameters. By inverting this reasoning, it should be possible to choose such values of material parameters which would make its reflectivity arbitrarily close to zero. It should be possible to achieve theoretically, by solving eq.(20). Stating eq.(20) in the form \( R(x) = 0 \), where \( x = K\omega/\pi\sigma_R \) leads to the value \( x = 0.744875 \). This idea will be pursued further elsewhere.

**Acknowledgments**

This paper was prepared within the research project 174031 financed by the Ministry of Education and Science of Serbia. The author is grateful to Dr. Steve Reynolds from the University of Dundee for his help in proofreading the paper.

**References**

[1] Mott N 1982 *Proc.R.Soc.London* A **382** 1
[2] Mott N 1968 *Rev Mod Phys.* **40** 677
[3] Hubbard J 1963 *Proc R Soc London* A **276** 238
[4] Lieb E H and Wu F Y 1968 *Phys Rev Lett* **20** 1445
[5] Mahan G D 2000 *Many-Particle Physics,third edition* (New York:Kluwer Academic/Plenum Publishers)p 24
[6] Celebonovic V in 2006, *Trends in Materials Science Research*, Editor Caruta B M, Nova Science Publishers Inc.,New York,pp.245-260
[7] Celebonovic V 2010 *J Phys Conf Ser* **253** 012004
[8] Wallis R F and Balkanski M 1986 *Many-Body Aspects of Solid State Spectroscopy* Amsterdam:North Holland
[9] van den Brink J 2006 *Nature Materials* **5** 427
[10] Jerome D 2012 *J Supercond Nov Magn* **25** 633
[11] Bourbonnais C and Sedeki A 2011 *C R Physique* **12** 532
[12] Nair R R, Blake P, Grigorenko A N, Novoselov K S, Booth T J, Struber T, Peres N M R and Geim A K 2008 *Science* **320** 1308
[13] Zhang B,Luo Y, Liu X and Barbastathi G 2011 *Phys Rev Lett* **106** 033901