# 2D Metal Insulator Transition: Calculation of Electrostatic Potential in Wigner-Seitz Cell

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The overall goal for this project is to describe the 2D-MIT as melting of the Wigner crystal and to develop a *microscopic* model. A first step for developing this theory is the calculation of the potential energy in a Wigner crystal, since the potential energy dominates at low density. To perform this calculation, we use the Ewald summation method. As a result, we have calculated the confining potential experienced by the lattice site, as well as for the additional interstitial sites. Additionally, we have created 2D and 3D plots to quantify our results, from which we learn the deep confining potential well on which the reference electron sits, on the scale $\frac{e^2}{a}$, is more than an order of magnitude larger than the potential well describing the interstitial site. We find the interstitial electron can be described as a nearly-free electron model, and the lattice electron by a tight-binding (localized orbital) model.

## I. INTRODUCTION

The central goal of materials science is designing and fabricating new materials with interesting transport, optical, and thermal properties. Most of these materials are neither good metals (conductors), nor good insulators; however, because of thermal fluctuations, every material has a finite, but often small, range of conductivity at nonzero temperature. Metal-insulator transitions (MIT) occur when the behavior of the material changes from the one characteristic for conductor (resistivity decrease with decreasing temperature,) to the behavior characteristic for an insulator. Systems that go through the MITs are some of the most studied materials in condensed matter physics (e.g. high-temperature super conductors, manganites, and doped semiconductors.)

In the past, there has been much success in describing the behavior of metals, insulators, and MIT using models based on weakly interacting electrons[1]. Based on the filling of the electronic band, this theory describes insulators having a completely filled band, and a metal, having the Fermi energy lie inside the band. However, there are many materials that according to the simple band picture of weakly interacting electrons should be a good conductor, but have very low conductivity. Such an example would be a Mott insulator[2], observed in 2D metal-oxide semiconductor field-effect transistor (MOSFETs) systems, whose strong repulsion of electrons affects the metallic/insulating behavior of the material. One other such theory, which poses additional conflicting ideas with the weakly interacting band theory, is Anderson localization[3]. Here, strongly disordered systems cause the wave functions to become bounded or localized, increasing the observed insulating behavior. Despite the prevailing success of models based on noninteracting electrons, an adequate, unifying microscopic theory of MIT is still missing.

With the latter thought in mind, it is the work of Dobrosavljević (*et al.,*) to formulate a comprehensive unifying theory in which the strong electron interactions and disorder are accounted for. It is here, in such a theory, that the calculation of potential energy in a Wigner lattice becomes an initial step.Throughout the remainder of this paper, the derivation, results, and conclusion of this calculation will be developed.

## II. MODELING THE 2D MIT

In the low density regime, 2D electrons form the Wigner crystal[4,5]. In this case, the electrons may be treated within the tight-binding model, as localized orbitals belonging to the sites of the triangular lattice. The overlap of the adjacent orbitals form the lower energy band. As the density is increased, the electron-electron interactions prevent the double occupancy of the lattice sites. In the case of half filling, the only possible energetically favorable state the electron can hop to are the interstitial sites; this forms the higher energy band. This two band model permits, in the high density regime, electron behavior to be modeled as a nearly-free electron model. It is easy to see from Fig.1 and Fig. 2 the two distinct energy bands as the electron "zig-zags" from the lattice site to the interstitial site.

This method of electron transport is due to the Coulomb interactions between the electrons, and it here that the calculation of the Coulomb potential becomes significant.

### A. Classical Calculation of Coulomb Potential in a Wigner Lattice

Because of the periodicity of the Wigner lattice, calculating the Coulomb potential yields itself well to Fourier analysis. More explicitly, the Wigner lattice potential satisfies the conditions $\phi(\mathbf{r}) = \phi(\mathbf{r} + \mathbf{R})$ where $\mathbf{r}$ is the

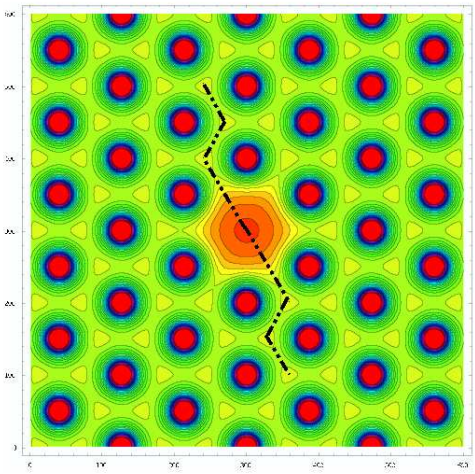

FIG. 1: 3D contour plot in 2D of Wigner lattice.Schematically represents the "zig-zag" path of the electron from the lattice site to the interstitial site.

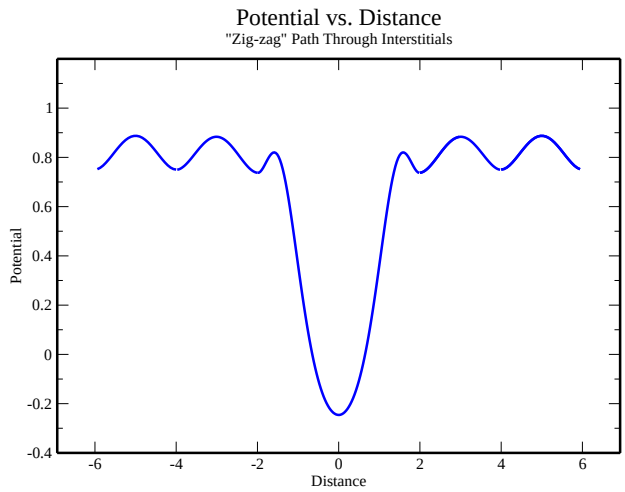


FIG. 2: 2D plot of Potential vs. Distance, where the scale is $\frac{e^2}{a}$.This plot qualitatively describes the "zig-zag" path an electron would take to hop from the lower energy band to the upper band (i.e. interstitial site.

position vectors (1) and **R** is the translation vector (2):

$$\mathbf{r} = x\hat{\mathbf{e_x}} + y\hat{\mathbf{e_y}} \tag{1}$$

$$\mathbf{R} = R_x\hat{\mathbf{a_1}} + R_y\hat{\mathbf{a_2}} \tag{2}$$

where

$$\mathbf{a_1} = (\frac{3^{1/2}}{2})\hat{\mathbf{x}} + (\frac{1}{2})\hat{\mathbf{y}}$$

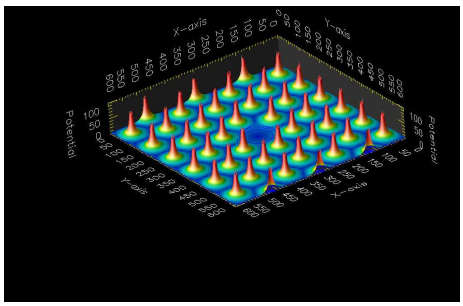

FIG. 3: 3D plot of Potential vs. X vs. Y

$$\mathbf{a_2} = -(\frac{3^{1/2}}{2})\hat{\mathbf{x}} + (\frac{1}{2})\hat{\mathbf{y}}$$

and $R_x$,$R_y$ are integers. To construct the Wigner lattice potential,we calculate the potential $\phi(\mathbf{r})$ at position **r** within an infinite lattice:

$$\phi(\mathbf{r}) = \sum_{i=1}^{\infty} \frac{q_i}{|\mathbf{r} - \mathbf{r_i}|} \tag{3}$$

To ensure charge neutrality,a positive background distribution is applied so that

$$\sum_{i}^{\infty} q_i = 0$$

. This poses a problem, however, for (3) is a divergent sum in the as i $\rightarrow \infty$.To resolve this, we employ a method developed by Ewald[6] and extended by Parry[7] to 2D, where the results are as follows:

$$\phi(\mathbf{r}) = \frac{2\pi}{\mathrm{A}} \sum_{\mathbf{G}\neq 0} \mathrm{G}^{-2}\exp(\imath\mathbf{G}\cdot\mathbf{r})\mathrm{erfc}(\frac{\mathrm{G}}{2\sqrt{\eta}}) + \sum_{\mathbf{R}} \mathrm{erfc}(\frac{\sqrt{\eta}|\mathbf{r}-\mathbf{R}|}{|\mathbf{r}-\mathbf{R}|}) - \frac{1}{\mathrm{A}}\sqrt{\frac{\pi}{\eta}} \tag{4}$$

where **G** is the reciprocal lattice vector, A is the area of the Wigner-Seitz cell, and $\sqrt{\eta}$ is a parameter chosen to obtain rapid convergence of both the lattice summations in (4).

## III. RESULTS

We have calculated the confining potential experienced by the lattice sites, as well as for the additional interstitial sites. Using XmGRACE and OpenDX, we have created detailed 2D and 3D pictures quantifying our results Fig. 1-3, from which we learned that the "big" potential well, of the lattice electron, sits is a deep confining well on the scale $\frac{e^2}{a}$. Additionally, we can observe the potential well describing the interstitial site (electron) is much shallower than the lattice site, by more then an order of magnitude.

## IV. CONCLUSION

We conclude that the interstitial electron can be described as a nearly-free electron model, while the lattice electron by a tight-binding (localized orbital) model.

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[1] N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Saunders, Philadelphia, 1976).

[2] N. F. Mott, *Metal-insulator transitions* (Taylor and Francis, London, 1947).

[3] P. W. Anderson, Phys. Mod. Phys . **50**, 191 (1978).

[4] B. Tanatar and D. M. Ceperley, Phys. Rev. B **39**, 5005 (1989).

[5] S. T. Chui and B. Tanatar, Phys. Rev. Lett. **74**, 458 (1995).

[6] P. P. Ewald, Ann. Physik. (Leipzig) **64**, 253 (1921).

[7] D. E. Parry, Surf. Sci. **49**, 433 (1976).