GENERALIZED WIGNER LATTICES AS A RIEMANN SOLID: FRACTALS IN THE HURWITZ ZETA FUNCTION

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We study the ground state configuration and the excitation energy gaps in the strong coupling limit of the extended Hubbard model with a long-range interaction in one dimension. As proved by Hubbard and Pokrovsky and Uimin, the ground state configuration is quasiperiodic and as proved by Bak and Bruinsma, the excitation energy has a finite gap which forms a devil's stair as a function of the density of particles in the system. We show that the quasiperiodicity and the fractal nature of the excitation energy come from the nature of the long-range interaction that is related to the fractal nature of the Hurwitz Zeta function and the Riemann Zeta function.

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1. Introduction
In this paper, we study why the quasiperiodicity and the fractal nature appear in the ground state and excitations in the strong coupling limit of a class of Hamiltonians that support the generalized Wigner crystallization in one dimension. We show that its origin comes from the mathematical properties of the Hurwitz Zeta function as well as Riemann Zeta function that is implicitly inherent in the theory. Hence, we can recognize the generalized Wigner lattices as a Riemann solid.

2. Calculation
The Hamiltonian that we study is that for spinless fermions with long-range interaction:

\[ H = -t \sum_{j=1}^{N} \{ c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1} \} + \sum_{1 \leq i < j}^{N} V_{|i-j|} n_i n_j , \]

where we assume that the condition

\[ 2V_n \leq V_{n+1} + V_{n-1} , \]

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is satisfied and \( V_n > 0 \) for all \( n \geq 1 \) with \( V_n \to 0 \) as \( n \to \infty \). This Hamiltonian was first studied by Hubbard,\(^3\) about twenty years ago, and it is now called the extended Hubbard model (without the on-site Coulomb interaction of \( U \to \infty \)). Denote the form of the potential by \( V_n = V \phi(x) \), where \( V \) is the coupling constant. We consider the Hamiltonian in the strong coupling limit of \( V \gg t \) such that we can neglect the hopping energy term. Therefore, we consider the following Hamiltonian:

\[
H = V \sum_{1 \leq i < j} \phi(|i - j|) n_i n_j = V \sum_{1 \leq i < j} \phi(|i - j|) .
\]

The ground state of this Hamiltonian was once studied by Hubbard,\(^3\) Pokrovsky and Uimin,\(^4\) and Bak and Bruinsma,\(^5\) and recently, by Sutherland\(^6\) and Hatsugai.\(^7\)

Assume that the system is a periodic lattice with \( N \) sites and consists of \( M \) particles so that the density is given by \( \rho = \sum_j n_j/N = M/N \). Minimizing the energy (3), Hubbard\(^3\) and Pokrovsky and Uimin\(^4\) showed that in the ground state arrangement of the particles, the position of the \( j \)th particle from the origin is given by

\[
x_j = \left[ \frac{j}{\rho} \right] ,
\]

where \( \left[ \right] \) represents the Gauss symbol that takes the largest integer part. This provides a periodic (commensurate) arrangement of the particles on the lattice if \( \rho \) is rational and a quasiperiodic (incommensurate) arrangement of the particles on the lattice with two-distance property if \( \rho \) is irrational.\(^8,9\) In Fig. 1, we show the ground state arrangement of the sites as a function of the density \( \rho \), which was first drawn by Iguchi.\(^8\)

As was proved by Hubbard,\(^3\) the above configuration is determined by the following algorithm:

(i) Define the density \( \rho = m/n \) (\( m, n \) are integers with no common factor).

(ii) Define the integers \( k, n_0, n_1, \ldots, n_k \) by the equations

\[
\begin{align*}
\frac{1}{\rho} &= n_0 + r_0 , \\
\left[ \frac{1}{r_0} \right] &= n_1 + r_1 , \\
\vdots & \\
\left[ \frac{1}{r_{k-2}} \right] &= n_{k-1} + r_{k-1} , \\
\left[ \frac{1}{r_{k-1}} \right] &= n_k ,
\end{align*}
\]

where for all \( s, -1/2 < r_s \leq 1/2 \) (the sequence must terminate for rational \( \rho \)).
Fig. 1. The quasiperiodic lattice order. The particles (holes) are shown by black (white) dots, where the position of the jth particle is exactly given by \( x_j = [j/\rho] \). The horizontal axis represents the density of particles \( \rho \), while the vertical axis represents the lattice sites in the system, where 301 sites are drawn.

(iii) Define the sequences \( X_1, X_2, \ldots, X_k \) and \( Y_1, Y_2, \ldots, Y_k \) by

\[
\begin{align*}
X_1 &= n_0, \\
Y_1 &= n_0 + \alpha_0, \\
\vdots \\
X_{i+1} &= [X_i]^{n_i-1}Y_i, \\
Y_{i+1} &= [X_i]^{n_i+\alpha_i-1}Y_i,
\end{align*}
\]

where \( \alpha_i = r_i/|r_i| = \pm 1 \). Then, \( X_k \) represents the unit cell of the system.

Equation (6) provides a symbolic sequence of 0 and 1. For example, if \( \rho = 1/2 \), then \( X_1 = 2, r_0 = 0 \) that represents \( X_1 = \text{"2"} \), which represents the system is \text{"101010\ldots"}, and if \( \rho = 2/5 \), then \( X_1 = 3, n_0 = 2, \alpha_0 = -1, Y_0 = 2 \) and \( X_2 = \text{"32"}, \) which means the system is \text{"1001010010\ldots"}. When \( \rho \) is irrational, the size of the unit cell becomes arbitrarily large. And hence, the lattice is quasiperiodic.

Hubbard's algorithm is also equivalent to the algorithm that was studied by Pokrovsky and Uimin\(^4\) for the same problem and by Iguchi\(^8\) and Sutherland\(^9\) for the theory of one-dimensional quasiperiodic lattices. We note that in the latter, the above scheme was successfully used to obtain the spectrum of electrons or photons.
in the quasiperiodic lattice using the so-called *trace map method*.\textsuperscript{8,10} The spectrum is a Cantor-set type while its wave functions are self-similar or fractal.

Let us consider the ground state energy and the excitations. The ground state energy is given by

\[ E_0(M) = M\mu + MV \sum_{k=0}^{\infty} \{(1 - f_k)\phi(d_k) + f_k\phi(d_k + 1)\}, \]

where \( d_k = |k/\rho| \) is the \( k \)th nearest neighbor distance and \( f_k = k/\rho - |k/\rho| \) such that \( d_k \leq k/\rho < d_k + 1 \) and \( \mu \) is the chemical potential for a particle. Following Bak and Bruinsma,\textsuperscript{5} we can obtain the excitation energy (the charge gap) of the system. The phase characterized by \( \rho = m/n \) is stable as long as it costs energy to add one more particle to the system or remove one particle from the system, and rearrange the new configuration to minimize the energy. The energy cost is given by

\[ \mu(\rho \pm 0) \equiv E_0(M \pm 1) - E_0(M) \equiv \mu_{\pm} \]

\[ = \pm \mu + V \sum_{k=0}^{\infty} \{ (d_k + 1)\phi(d_k) - d_k\phi(d_k + 1) \}, \]

where \( d_p = n \) for \( \mu_+ \) and \( d_p = n - 1 \) for \( \mu_- \). Therefore, the interval where the phase is stable is determined by \( \mu_{\pm} = 0 \), respectively. This yields the charge gap

\[ \Delta\mu(\rho = m/n) = \mu_+ - \mu_- \]

\[ = V \sum_{k=1}^{\infty} nk[\phi(nk + 1) + \phi(nk - 1) - 2\phi(nk)]. \]

Since \( \phi(x) \) satisfies the condition (2), the right hand side of (9) is positive definite. Hence, the excitation has a finite gap.

Suppose the form of the potential is

\[ \phi(x) = \frac{1}{x^s}. \]

The calculation of (9) with (10) has been carried out numerically for the special value of \( s = 2 \). It was first studied by Bak and Bruinsma\textsuperscript{5} and recently studied by Hatsugai\textsuperscript{7}. The other cases have not been well-known so far, since the difficulty in the calculation of the infinite sum, however. When we plot \( \Delta\mu \) as a function of \( \rho \), this expression includes a very complicated and beautiful *devil’s stair*-like function.\textsuperscript{5,7} It may also be relevant to explain the *magnetization plateau problem*,\textsuperscript{3} regarding \( \mu \) and \( \rho \) as \( H \) the external magnetic field and \( m \) the magnetization, respectively.

Now, we are going to represent (9) in terms of the Hurwitz Zeta function\textsuperscript{3} as

\[ \zeta(s/a) = \sum_{l=0}^{\infty} \frac{1}{(l+a)^s}. \]
Substituting (10) into (9) and using (11), we find the following:

\[ \Delta \mu \left( s|\rho = \frac{m}{n} \right) = \frac{V}{n^{s-1}} f(s-1|\rho), \quad (12) \]

where we have defined as

\[ f(s-1|\rho) \equiv \zeta \left( s-1|1+\frac{1}{n} \right) + \zeta \left( s-1|1-\frac{1}{n} \right) - 2\zeta(s-1|1) \]

\[ -\frac{1}{n} \left[ \zeta \left( s|1+\frac{1}{n} \right) - \zeta \left( s|1-\frac{1}{n} \right) \right] \]

and

\[ \zeta(s|1) = \zeta(s) = \sum_{i=1}^{\infty} \frac{1}{i^s}, \quad (14) \]

the Riemann Zeta function.\(^2\)

The advantage of the above expression (12) is the following:

1. First, the convergence of the Hurwitz Zeta function is well-known.\(^2\)
2. Second, once we write the expression, the origin of the singular nature is transparent; it comes only from \( f(s-1|\rho) \). In other words, the fractal nature comes from the Hurwitz Zeta function as well as the Riemann Zeta function.
3. Third, we can treat not only the case of \( s = 2 \) but also the other cases of arbitrary \( s \).
4. Fourth, the devil's stair like function is given by the sum

\[ F\left( s-1|\rho = \frac{m}{n} \right) = \sum_{k=1}^{M} f \left( s-1|\rho = \frac{k}{N} \right), \quad (15) \]

where \( \rho = M/N = m/n \). Thus, we can conclude that all the known results in the previous works can be obtained from the knowledge of the function, \( f(s-1|\rho) \). And it enables us to treat the problem not only numerically, but also analytically. To show the above points, we show that the universal fractal nature of the function, \( f(s-1|\rho) \) in Fig. 2, and the devil's stair like function \( F(s-1|\rho) \) in Fig. 3.

Let us consider (12) in the incommensurate limit when \( \rho \) becomes irrational such that \( \rho = m/n \to \text{const.} \) with \( m \to \infty \) and \( n \to \infty \). In this limit, from (13), we find that

\[ f(s-1|\rho) = \frac{1}{n^2} \left[ \frac{\partial^2}{\partial a^2} \zeta(s-1|a) - 2 \frac{\partial}{\partial a} \zeta(s|a) \right]_{a=1} + O \left( \frac{1}{n^3} \right). \quad (16) \]

From the properties of the Hurwitz Zeta function (11), we prove unless \( s = 0 \)

\[ \frac{\partial^k}{\partial a^k} \zeta(s|a) = (-1)^k s(s+1) \cdots (s+k-1) \zeta(s+k|a). \quad (17) \]
Fig. 2. The fractal nature of the function, $f(s - 1|\rho)$. The horizontal axis represents the density of particles $\rho$, while the vertical axis represents the magnitude of the function. The vertical axis is normalized by the units of $\frac{f(s - 1|1/2)}{s}$. Two cases of $s = 2, 5$ are shown. As the value of $s$ is increased, the damping becomes faster.

Using (17) in (16), we find

$$f(s - 1|\rho) = \frac{s(s + 1)}{n^2} \zeta(s + 1) + O \left( \frac{1}{n^3} \right).$$

(18)

Therefore, from (12) we obtain

$$\Delta \mu(s) = \frac{V}{n} \frac{s(s + 1)}{n^{s+1}} \zeta(s + 1) + O \left( \frac{1}{n^{s+2}} \right) \xrightarrow{n \to \infty} 0,$$

(19)

where $\zeta(s)$ is a constant if $s$ is real. For example, if $s = 2$ as is in the Bak and Bruinsma case, then we find $\Delta \mu(2) = \frac{6V\zeta(3)}{n^3} + O \left( \frac{1}{n^4} \right) \to 0$ as $n \to 0$. Thus, the excitation energy gap vanishes when $\rho$ is irrational.
3. Conclusion

In conclusion, we have studied the ground state and the excitation energy gaps in the strong coupling limit of the Hamiltonian with long-range interaction in one dimension. The ground state is realized as generalized Wigner lattices with a quasiperiodic particle order. When the density is fractional, the excitation energy has a finite gap from the ground state and the lattice is a commensurate order. And when the density is irrational, the excitation energy has no gap and the lattice is a quasiperiodic order. The excitation energy gap forms a devil's stair-like function as a function of the density. We have shown that the quasiperiodicity of the lattice structure and the fractal nature of the excitation gaps come from the nature of the long-range interaction in the Hamiltonian, which is dominated by the nature of the Hurwitz Zeta function and the Riemann Zeta function. Thus, we conclude that the generalized Wigner lattice can be called a Riemann solid, that is, a solid whose physical properties are essentially governed by the mathematical properties of the Riemann Zeta function.

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References