Title?

Adam Kłosiński¹, Piotr Wrzosek¹, Cliò Agrapidis^{1,2}, and Krzysztof Wohlfeld¹

¹Institute of Theoretical Physics, Faculty of Physics,

University of Warsaw, Pasteura 5, PL-02093 Warsaw, Poland

(Dated: August 22, 2020)

Abstract...

I. INTRODUCTION

- 1. Considering the t- J^z model on the Bethe lattice is similar to harmonic approximation to hydrogen atom problem. In both cases the particle (either hole or electron respectively) is confined in the infinite potential (either close to linear or quadratic respectively). This results in ladder-like energetic structure of the problem (with either decreasing or equal gaps respectively).
- 2. But for the same problem on e.g. the 2D square lattice the confining potential does not have to be linear. There are two differences. First is related to Trugman processes (hole walking in a loop) possible in a square lattice: The hole propagates to e.g. next-nearestneighbour site in a process similar to tunnelling over a potential barrier. It leads to small momentum dependence in the spectral function of the hole. Second is more interesting and it is related to warping of the potential due to partial refinement of the antiferromagnetic order when hole moves along tangential paths (or at least partially tangential paths). Effectively the potential acts on the hole rather locally due to flattening with the distance. This behaviour is similar to taking into account the anharmonicity in the hydrogen atom problem. In the end the spectrum of the problem in low energies consists of well defined energy levels while the electron may be excited to the vacuum (i.e. continuum of energies above the confining potential).
- 3. For the case of a single hole on the Bethe lattice it is possible to show that effectively the t- J^z model can be mapped onto non-interacting one, where each magnon (excluding maybe the first one) costs the same amount of energy. One can think of a generalization of the above allowing e.g. position dependent cost of creating a magnon in the system. This is similar to introducing anharmonicity to primarily harmonic potential. We show that analogy to anharmonic potential works (see figures 2-6, in particular 2 and 5), i.e. there is a continuum above a discrete spectrum. Of course we do not have continuum of states up to infinite energy but a finite bandwidth.
- 4. In continuous limit of the particle in external potential problem any arbitrary small potential in n < 3 dimension leads to an appearance of a bound state [cite]. In 3D and above the competition between confining potential and the delocalization of the particle can be

won in favour of the latter for a finite confining potential. Interestingly we show that on the Bethe lattice this behaviour is reproduced already for z=3, see Fig. 1, while for the point potential in 1D (i.e. z=2, what exactly corresponds to the t- J^z model) we always see a QP in the spectral function of a single hole for any J>0.

II. MODEL

We consider the following model on the Bethe lattice

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} \left[h_i^{\dagger} h_j \left(a_i + a_j^{\dagger} (1 - a_i^{\dagger} a_i) \right) + h_j^{\dagger} h_i \left(a_j + a_i^{\dagger} (1 - a_j^{\dagger} a_j) \right) \right] + \sum_i J_i a_i^{\dagger} a_i,$$

$$\tag{1}$$

describing hopping of a hole (h_i) on the lattice accompanied by creation or annihilation of magnons (a_i) . We calculate the spectral function,

$$A(\omega) = -\frac{1}{\pi} \text{Im} \left(G(\omega + i0^+) \right) \tag{2}$$

of a single hole in such system. States with both hole and the magnon at the same site are projected out $(1-a_i^{\dagger}a_i)$. In general, the model describes the problem of a particle travelling through the lattice and exciting/relaxing the lattice by an amount of energy dependent on the position of the particle.

A. Relation to the t- J^z model

For constant $J_i \propto J$ the above model is an approximation of the t- J^z model with a single hole,

$$\mathcal{H}_{t-J^z} = -t \sum_{\langle i,j \rangle, \sigma} \left(\tilde{c}_{i\sigma}^{\dagger} \tilde{c}_{j\sigma} + \text{H.c.} \right) + J \sum_{\langle i,j \rangle} \left(S_i^z S_j^z - \frac{1}{4} \, \tilde{n}_i \tilde{n}_j \right),$$
(3)

expressed in terms of hole and magnon operators with potential energy proportional to J treated within the linear spin wave (LSW) theory. The transformation starts with the rotation of spins on one sublattice

$$\mathcal{H}_{\text{rot}} = -t \sum_{\langle i,j \rangle, \sigma} \left(\tilde{c}_{i\sigma}^{\dagger} \tilde{c}_{j\bar{\sigma}} + \text{H.c.} \right) - J \sum_{\langle i,j \rangle} (S_i^z S_j^z + \frac{1}{4} \tilde{n}_i \tilde{n}_j).$$

$$\tag{4}$$

It allows for introduction of holes and magnons in terms of following transformations,

$$\begin{aligned}
\tilde{c}_{i\uparrow}^{\dagger} &= h_i, & \tilde{c}_{i\uparrow} &= h_i^{\dagger} (1 - a_i^{\dagger} a_i), \\
\tilde{c}_{i\downarrow}^{\dagger} &= h_i a_i^{\dagger}, & \tilde{c}_{i\downarrow} &= h_i^{\dagger} a_i,
\end{aligned} (5)$$

$$S_i^z = \frac{1}{2} - a_i^{\dagger} a_i - \frac{1}{2} h_i^{\dagger} h_i,$$

$$\tilde{n}_i = 1 - h_i^{\dagger} h_i.$$
(6)

Then, kinetic energy in terms of hole and magnon operators reads,

$$\mathcal{H}_{t} = -t \sum_{\langle i,j \rangle} \left[h_{i}^{\dagger} h_{j} \left(a_{i} + a_{j}^{\dagger} (1 - a_{i}^{\dagger} a_{i}) \right) + h_{j}^{\dagger} h_{i} \left(a_{j} + a_{i}^{\dagger} (1 - a_{j}^{\dagger} a_{j}) \right) \right].$$

$$(7)$$

Accordingly, the potential energy reads,

$$\mathcal{H}_{J} = E_{0} + \frac{J}{2} \sum_{\langle i,j \rangle} \left[a_{i}^{\dagger} a_{i} + a_{j}^{\dagger} a_{j} - 2 a_{i}^{\dagger} a_{i} a_{j}^{\dagger} a_{j} + h_{i}^{\dagger} h_{i} + h_{j}^{\dagger} h_{j} - h_{i}^{\dagger} h_{i} a_{j}^{\dagger} a_{j} - h_{j}^{\dagger} h_{j} a_{i}^{\dagger} a_{i} - h_{i}^{\dagger} h_{i} h_{j}^{\dagger} h_{j} \right].$$

$$(8)$$

Neglecting constant energy shift, magnon-magnon interactions (LSW) and terms related to the holes (which do not play qualitative role assuming there is a single hole in the system) one ends up with the model stated in Eq. 1 with J_i constant.

III. BETHE LATTICE

A. Methods

In a case of the Bethe lattice with coordination number z one can obtain a convenient basis of states reachable from initial state $|0\rangle$, that tridiagonalizes the matrix of the model Hamiltonian in the reachable subspace. The initial state $|0\rangle$ is a state without magnons with a single hole located at the origin, i.e. at site i = 0. The number of possible states that can be achieved with a single hop of a hole is equal to the coordination number z, so there are z reachable states with one magnon. We denote the normalized sum of those as $|1\rangle$. Similarly, there are z(z-1) states with 2 magnons. The factor z-1 comes from the fact that once hole leaves the origin then one site in the proximity of a hole is occupied by a magnon. Normalised sum of reachable states with 2 magnons is denoted as $|2\rangle$. For n>0 there are $z(z-1)^{n-1}$ reachable states with normalised sum denoted as $|n\rangle$. In basis $\mathcal{B} = (|0\rangle, |1\rangle, |2\rangle, ...)$ the matrix of the Hamiltonian appears tridiagonal,

$$\mathcal{M}(\mathcal{H}) = \begin{bmatrix} V_0 & -t\sqrt{z} \\ -t\sqrt{z} & V_1 & -t\sqrt{z-1} \\ -t\sqrt{z-1} & V_2 & -t\sqrt{z-1} \\ & -t\sqrt{z-1} & V_4 & \ddots \\ & & \ddots & \ddots \end{bmatrix},$$
(9)

where $V_i = \sum_{k=0}^{i-1} J_k$. This yields a simple formula for the Greens function in a form of a continued fraction,

$$G(\omega) = \left\langle 0 \left| \frac{1}{\omega - \mathcal{H}} \right| 0 \right\rangle = \frac{1}{\omega - V_0 - \Sigma(\omega)},$$
 (10)

where the corresponding expression for self-energy appears as follows,

$$\Sigma(\omega) = \frac{zt^2}{\omega - V_1 - \frac{(z-1)t^2}{\omega - V_2 - \dots}}.$$
 (11)

B. Point Potential Results

In particular, we study the problem of a single hole on the Bethe lattice in the case of a point potential located at the origin (i.e. in the position where the hole was created in the system). It corresponds to $J_i = V$, when i = 0 and $J_i = 0$ otherwise. This leads to the following expression for the self-energy,

$$\Sigma(\omega) = \frac{zt}{z-1} \left(\frac{\omega - V}{2t} \pm \sqrt{\left(\frac{\omega - V}{2t}\right)^2 - (z-1)} \right). \tag{12}$$

From the above on can easily calculate the analytic formula for the quasiparticle residue z_0 and the limiting value V^* for which the system undergoes transition form having to not having quasiparticle solution.

$$z_0(z, t, V) = \lim_{\omega \to \omega^*} (\omega - \omega^*) G(\omega) = \lim_{\omega \to \omega^*} \frac{1}{1 - \frac{d}{d\omega} \Sigma(\omega)}$$

$$= \left(\frac{z - 2}{2(z - 1)} + \frac{1}{\sqrt{1 - \frac{16t^2(z - 1)}{((z - 2)V - z\sqrt{V^2 + 4t^2})^2}}} \right)^{-1},$$
(13)

$$V^*(z,t) = t \frac{z-2}{\sqrt{z-1}}. (14)$$

C. Arbitrary Potential Shape

Let us consider more general case. Now we take arbitrary shape of the on site potential V_k , where k

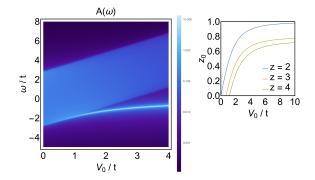


FIG. 1: Spectral function of a single hole for various strengths of a point potential V_0 and coordination number z=3 (left) and quasiparticle residue $z_0(V_0)$ for few coordination numbers z (right). In the figure of the spectral function (left) the transition occurs at $V_0 = \frac{t}{\sqrt{2}} \approx 0.7t.$

stands for the distance from the origin. Let us denote $\Gamma(\omega) = \frac{(z-1)t^2}{\omega - V - \Gamma(\omega)}$, $\Omega_k = \omega - V_{k < n}$, $\Omega_n = \frac{(z-1)t^2}{\Gamma(\omega)}$, $\tau_1 = zt^2$ and $\tau_{k>1} = (z-1)t^2$. Then we can write down the expression for the self-energy as follows,

$$\Sigma(\omega) = \frac{\tau_1}{\Omega_1 - \frac{\tau_2}{\Omega_2 - \frac{\tau_3}{\Omega_2 - \dots}}} = \frac{z}{z - 1} \mathop{\mathcal{K}}_{k=1}^n \left(\frac{\tau_2}{\Omega_k}\right). \tag{15}$$

In order to obtain the expression for the quasi-particle residue

$$z_0 = \lim_{\omega \to \omega^*} \frac{1}{1 - \frac{d}{d\omega} \Sigma(\omega)},\tag{16}$$

we calculate the derivative of the self-energy with respect to frequency ω ,

$$\frac{d}{d\omega}\Sigma(\omega) = \frac{z}{z-1}\frac{d}{d\omega} \mathop{\mathcal{K}}_{k=1}^{n} \left(\frac{\tau_2}{\Omega_k}\right) =
= \frac{z}{(z-1)^2 t^2} \sum_{j=1}^{n} (-1)^{j+1} \prod_{k=1}^{j} \left[\mathop{\mathcal{K}}_{l=k}^{n} \left(\frac{\tau_2}{\Omega_l}\right)\right]^2 \frac{d\Omega_j}{d\omega},$$
(17)

where $\frac{d}{d\omega}\Omega_{j< n} = 1$ and $\frac{d}{d\omega}\Omega_n = \frac{d}{d\omega}\left(\frac{(z-1)t^2}{\Gamma(\omega)}\right)$. Note, V^* is not well defined in general, so we do not provide any expression here.

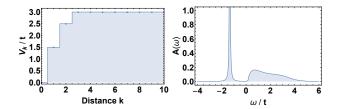


FIG. 2: Shape of the potential V_k confining the hole (left) and the spectral function of a single hole (right) for $J_{k\in\{0,1,2\}} = (\frac{3}{2} - \frac{k}{2})t$ and $J_{k>2} = 0$. Coordination number z = 3. The quasiparticle solution is well separated from the continuum.

D. Linear Potentials

In what follows we investigate properties of the spectral function of a single hole for linearly shaped potentials. Further analysis includes four cases:

- (i) constant area enclosed by the linear potential well with the width of the well changing (Fig. 3),
- (ii) constant depth of the well with the width varying (Fig. 4),
- (iii) constant width with varying depth (Fig. 5),
- (iv) constant slope of the well for various width of the well (Fig. 6).

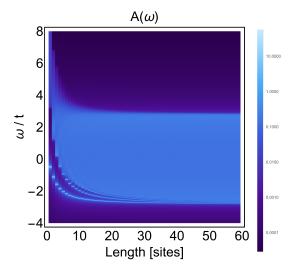


FIG. 3: Spectral function of a single hole for constant 'area' of the potential A=6t. Coordination number z=3. Transition from single quasiparticle (through multiple QPs) into a continuum is observed.

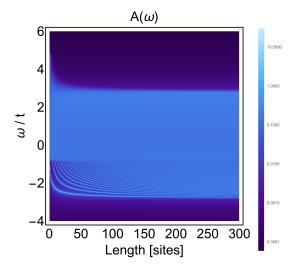


FIG. 4: Spectral function of a single hole for constant potential depth $V_0 = 2t$. Coordination number z = 3. Dependent on the V_0 transition from no QP to single QP and then through multiple QPs into a continuum can be observed.

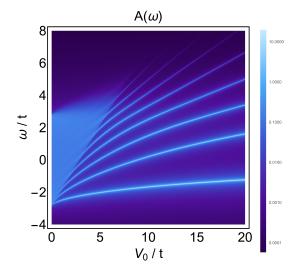


FIG. 5: (Spectral function of a single hole for constant 'half-width' of the well L=12 sites. Coordination number z=3. Transition from continuum into a multiple QPs is observed.

E. Discussion

In Figs. 3, 4 and, 6, spectrum at length of the well L=1 corresponds to vertical cross of the density map of the point potential case (Fig. 1). It is visible that

dependent on the point potential depth the solution may or may not contain the quasiparticle initially. Regardless of whether QP initially exists or not in all three cases (i), (ii) and, (iv) multiple peaks eventually appear when the

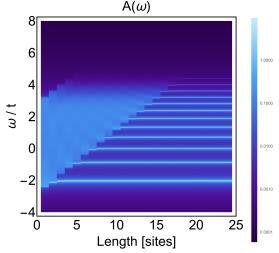


FIG. 6: Spectral function of a single hole for constant potential step J=0.4t. Coordination number z=3. Transition from continuum into a multiple QPs is observed resulting in t- J^z model solution on the Bethe lattice.

width of the well grows.

The range of energies where the quasiparticle solutions may exist corresponds to the depth of the potential well. For energies exceeding depth of the well potential there is always a continuum of states provided that well is not deeper than energy range covered by the continuum. This can be best visible in Fig. 4 of case (ii) where the depth of the well is constant, $V_0 = 2t$. Of course, for small widths of the well the ground state is not at the bottom so the range of energies that is covered by QP solutions seems smaller then actual depth of the well. In cases (i) and (ii), when the width of the well is rising more and more solutions fit in the well while distances between them get smaller and smaller. In the thermodynamic limit when the well totally disappears the continuum rebuilds. In case (iv) in thermodynamic limit the linear potential covers whole lattice, thus one reproduces known t- J^z model solution.

The case (iii) is different from others in that sense that it is the only case where the width of the well is constant. The vertical cross of Fig. 5 at $V_0 = LJ = 4.8t$ is equal to the vertical cross through Fig. 6 at length L = 12 (where J = 0.4t).