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REAL SPACE RENORMALIZATION GROUP FOR SPECTRA AND DENSITY OF STATES †

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ABSTRACT

We discuss the implementation of the Real Space Renormalization Group Decimation Technique for 1-d tight-binding models with long range interactions with or without disorder and for the 2-d regular square lattice. The procedure follows the ideas developed by Southern et al. Some new explicit formulae are included. The purpose of this study is to calculate spectra and densities of states following the procedure developed in our previous work,

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I. INTRODUCTION

Real space Renormalization Group (R-G) decimation technique is a useful method to calculate excitations and densities of states in tight-binding type of models [1]. The interest of the approach to this technique which we discuss here is in the fact that physical quantities are obtained from convergence properties of certain parameters upon renormalization (the on-site coefficients and the hoppings) without the need of specifying any particular boundary conditions. Of course for non-disordered problems the answers are well known and they are easily calculated by Fourier transformations. However it is interesting to see that in the R-G method the disordered case can be treated with exactly the same procedure as the ordered case and just the rescaling of the coefficients gives the correct answers in both cases.

Several physical systems of recent interest can be described by tight-binding models: crystals containing a modulating periodic potential of a period different from that of the underlying lattice, either commensurate or incommensurate with it [2]; electrons in 2-d square lattice in a perpendicular magnetic field [3]; the Schrödinger equation with an arbitrary potential of atomic type (through the construction of the Poincaré map of the problem [4]); superconductive networks (De-Gennes-Alexander theory [5]) etc.

The philosophy of the R-G is to change a problem with many degrees of freedom into another one with less degrees of freedom without losing any physical feature. We will limit ourselves here only to cases where this can be fulfilled without any approximation. Elimination of alternate sites (decimation) for 1-d models with nearest neighbours interactions with or without translational invariance is the simplest case that fulfills this [6),7),8),9)]. Southern et al. [10] showed that this also happens in 1-d with any range of interactions. We will discuss this case in more detail here. Decimation can also be performed exactly on fractals by eliminating sites belonging to alternate steps of formation of the fractal [11),12),13)]. Very recently Southern et al. [14] have succeeded in obtaining the prescription how to achieve the real space decimation in 2-d and 3-d lattices. However in these cases, upon renormalization, new longer range interactions are generated. They cut the process by working with a finite size portion of the lattice and show reasonably good results for pure cases. As we shall see in what follows, we have found, following their prescription, a general formula for the coefficients upon iteration up to any order for the pure 2-d lattice. This in principle could be extended to the disordered case but it is much more work consuming and at present we do not have any clear-cut results.

Summarizing, what we want to show here is the explicit formulation of the exact real space R-G decimation for 1-d longer than nearest neighbours interactions models with or without translational invariance and for the translationally invariant 2-d square lattice following the procedure recently studied by Southern et al. [10),14)] and adding some of our results.

We want to comment that once the Real space decimation is performed there are different ways of obtaining the physical quantities.. Both Gonçalves da Silva and Koiller [6] and Southern et al. [10] and our previous work [8),9),15)] are based on the convergence properties of the coefficients upon renormalization. They decimate the equation of motion for the Green function in real space and calculate densities of states by the usual relation with the imaginary part of the local Green function. Their procedure needs the use of small imaginary parts which sometimes give non-physical densities of states [15]. Besides their averaging procedure for disordered problems, although simple, means introducing an approximation which can also lead to only qualitative results. Our work is based on the equation of motion for the magnitude itself (wave-function, order parameter, spin, etc.) and we only deal with real numbers. The density of states is obtained from the poles of the real-part of the Green function (the on-site coefficient) [9),15)] and no approximations due to early averaging over configurations are introduced.

For ordered systems and for fractals a different approach was also developed and used [1),16),13)]. This is a one-parameter approach and is based on the scaling equation of the eigenvalue itself. Because of that it is called dynamical scaling. This has also been used for diluted magnetic systems by Stinchcombe [1] through the introduction of scaling laws for the probability distribution of bonds.

II. DECIMATION IN REAL SPACE

Within our procedure [6] we start with the equation of motion:

$$\varepsilon_m^{(o)} \psi_m - \sum_{\delta_i} \left[t^{(o)}_{m-\delta_i,\, m} \psi_{m-\delta_i} + t^{(o)}_{m,\, m+\delta_i} \psi_{m+\delta_i} \right] = 0 \quad ,$$

where ψ_n has the meaning of the wave-function, the order parameter, spin amplitude etc. and is the unknown magnitude to be calculated, ε_n is the on-site parameter (in fact it has to be understood as $\omega - \varepsilon_n$, ω being the eigenvalue which has also to be determined) and t is the off-diagonal parameter connecting sites at distance δ_i. The subscript zero means initial values of the parameters. Next the intermediate degrees of freedom are eliminated (each second site on the chain, each site n,m on the square lattice which has n+m = odd number) obtaining the equation of motion

for the bigger lattice and the corresponding relations. Upon repeating this procedure the lattice of even bigger spacing is reached (lattice constant = 2^r for 1-d , 2 to power r/2 for 2-d , r being the order of iteration) with the corresponding, form-conserving equation:

$$\epsilon_n^{(r)} \psi_n - \sum_{\delta_i} \left[t^{(r)}_{n-\delta_i, n} \psi_{n-\delta_i} + t^{(r)}_{n, n+\delta_i} \psi_{n+\delta_i} \right] = 0$$

with δ_i being the distance on the new lattice.

Let us explicitely show how to obtain the recursion relations through this elimination procedure.

(a) Pure 1-d chain with 1^{st} and 2^{nd} neighbours interactions and an explicit extension to any range of interaction. The original equation of motion reads:

$$\epsilon_n + t^1_{n+1} + t^1_{n-1} + t^2_{n+2} + t^2_{n-2} = 0 \quad .$$

In this notation n±i denotes the wave-function at a given site, $\epsilon = \omega - \epsilon$ and t^1 is the hopping on the nearest neighbour and t^2 on the next nearest neighbour. Next we write down the analogous equations for all the sites connected with the chosen one n (here, for the 1^{st} and 2^{nd} neighbours of n):

$$\begin{aligned}
&\epsilon_{n+1} + t^1_{n+2} + t^1_n + t^2_{n+3} + t^2_{n-1} = 0 \\
&\epsilon_{n-1} + t^1_n + t^1_{n-2} + t^2_{n+1} + t^2_{n-3} = 0 \\
&\epsilon_{n+2} + t^1_{n+3} + t^1_{n+1} + t^2_{n+4} + t^2_n = 0 \\
&\epsilon_{n-2} + t^1_{n-1} + t^1_{n-3} + t^2_n + t^2_{n-4} = 0 \quad .
\end{aligned}$$

Next, as we want to eliminate odd sites (n±1 , n±3), we multiply the equations for them (the first two) by minus their coupling constant that appears in the equation for site n divided by the on-site energy (namely by $-t^1/\epsilon$) and we multiply the rest by t^2/ϵ . Then we sum up the previous 4 equations with the first one for the chosen site n , we automatically cancel all the odd-sites and we are left with the equation for the doubled lattice (again with interactions only with 1^{st} and 2^{nd} neighbours on a new lattice). So we get:

$$\left[\epsilon - \frac{2(t^1)^2}{\epsilon} + \frac{2(t^2)^2}{\epsilon} \right] \psi_n + \left[2t^2 - \frac{(t^1)^2}{\epsilon} \right] \psi_{n+2} +$$

$$+ \left[2t^2 - \frac{(t^1)^2}{\epsilon} \right] \psi_{n-2} + \left[\frac{(t^2)^2}{\epsilon} \right] \psi_{n+4} + \left[\frac{(t^2)^2}{\epsilon} \right] \psi_{n-4} = 0 \quad .$$

So the recursion relations in this case are:

$$\left[\epsilon\right]^r = \left[\epsilon - \frac{2(t^1)^2}{\epsilon} + \frac{2(t^2)^2}{\epsilon} \right]^{r-1}$$

$$\left[t^1\right]^r = \left[2t^2 - \frac{(t^1)^2}{\epsilon} \right]^{r-1}$$

$$\left[t^2\right]^r = \left[\frac{(t^2)^2}{\epsilon} \right]^{r-1} \quad ,$$

where the exponent associated with the brackets means that the parameters should be taken at that iteration.

We have repeated this procedure for longer range interactions and we have noticed that there is a general law for the recursion relations of the different parameters as the range of the interaction is increased. Our result is:

$$\left[\epsilon\right]^r = \left[\epsilon - \frac{2(t^1)^2}{\epsilon} + \frac{2(t^2)^2}{\epsilon} - \frac{2(t^3)^2}{\epsilon} + \frac{2(t^4)^2}{\epsilon} - \frac{2(t^5)^2}{\epsilon} + \frac{2(t^6)^2}{\epsilon} \ldots \right]^{r-1}$$

$$\left[t^1\right]^r = \left[-\frac{(t^1)^2}{\epsilon} + 2t^2 - \frac{2t^1t^3}{\epsilon} + \frac{2t^2t^4}{\epsilon} - \frac{2t^3t^5}{\epsilon} + \frac{2t^4t^6}{\epsilon} - \frac{2t^5t^7}{\epsilon} \ldots \right]^{r-1}$$

$$\left[t^2\right]^r = \left[\frac{(t^2)^2}{\epsilon} - \frac{2t^3t^1}{\epsilon} + 2t^4 - \frac{2t^1t^5}{\epsilon} + \frac{2t^2t^6}{\epsilon} - \frac{2t^3t^7}{\epsilon} \ldots \right]^{r-1}$$

$$\left[t^3\right]^r = \left[-\frac{(t^3)^2}{\epsilon} + \frac{2t^2t^4}{\epsilon} - \frac{2t^1t^5}{\epsilon} + 2t^6 - \frac{2t^1t^7}{\epsilon} + \ldots \right]^{r-1}$$

$$\left[t^4\right]^r = \left[\frac{(t^4)^2}{\epsilon} - \frac{2t^3t^5}{\epsilon} + \frac{2t^2t^6}{\epsilon} - \frac{2t^1t^7}{\epsilon} \ldots \right]^{r-1}$$

$$\left[t^5\right]^r = \left[-\frac{(t^5)^2}{\epsilon} + \frac{2t^4t^6}{\epsilon} - \frac{2t^3t^7}{\epsilon} \ldots \right]^{r-1}$$

$$\left[t^6\right]^r = \left[\frac{(t^6)^2}{\epsilon} - \frac{2t^5t^7}{\epsilon} \ldots \right]^{r-1}$$

$$\left[t^7\right]^r = \left[-\frac{(t^7)^2}{\epsilon} \ldots \right]^{r-1} \quad .$$

Notice that the supraindex refers to the range of interaction at the lattice corresponding to the taken iteration.

(b) Disordered 1-d chain with 1^{st} and 2^{bd} neighbours interactions and formal extension to longer range interactions.

We start with the equation for a chosen site n :

$$\varepsilon_n + t^1_{n+1}\, n+1 + t^1_n\, n-1 + t^2_{n+2}\, n+2 + t^2_n\, n-2 = 0$$

with the convention that the supraindex accompanying the t's means the range of the interaction and the subindex means the biggest site it connects (e.g. t^1_{n+1} means the link between nearest neighbours n and n+1). In this way we take account of the fact that the link to the right between n and n+1 is the same as the link to the left between n+1 and n . Next we write down the equations for all the sites connected with n :

$$\varepsilon_{n+1}\, n+1 + t^1_{n+2}\, n+2 + t^1_{n+1}\, n + t^2_{n+3}\, n+3 + t^2_n\, n-1 = 0$$

$$\varepsilon_{n-1}\, n-1 + t^1_n\, n + t^1_{n-1}\, n-2 + t^2_{n+1}\, n+1 + t^2_{n-1}\, n-3 = 0$$

$$\varepsilon_{n+2}\, n+2 + t^1_{n+3}\, n+3 + t^1_{n+2}\, n+1 + t^2_{n+4}\, n+4 + t^2_{n+2}\, n = 0$$

$$\varepsilon_{n-2}\, n-2 + t^1_{n-1}\, n-1 + t^1_{n-2}\, n-3 + t^2_n\, n + t^2_{n-2}\, n-4 = 0 \ .$$

In this case we multiply each of these 4 equations by arbitrary constants which we call respectively $L^1(n+1)$, $L^1(n)$, $L^2(n+2)$, $L^2(n)$. Next we sum up all the 5 equations. We determine the constants by asking that the odd sites (n±1 , n±3) get eliminated, therefore imposing that the coefficients coresponding to them be zero. These conditions are:

$$t^1_{n+1} + L^1(n+1)\,\varepsilon_{n+1} + t^2_{n+1}\,L^1(n-1) + t^1_{n+2}\,L^2(n+2) = 0$$

$$t^1_n + L^1(n-1)\,\varepsilon_{n-1} + t^2_n\,L^1(n+1) + t^1_{n-1}\,L^2(n) = 0$$

$$t^1_{n+3}\,L^2(n+2) + t^2_{n+3}\,L^1(n+1) = 0$$

$$t^1_{n-2}\,L^2(n) + t^2_{n-1}\,L^1(n) = 0$$

By solving this system of equations we determine the 4 constants. Replacing them in the coefficients accompanying the even sites we get the explicit recurrence formulae. The recursion relations in this case are:

$$\left[\varepsilon_n\right]' = \left[\varepsilon_n + t^1_{n+k}\,L^1(n+k) + t^1_n\,L^1(n) + t^2_{n+2k}\,L^2(n+2k) + t^2_n\,L^2(n)\right]^{r-1}$$

$$\left[t^1_{n+k}\right]' = \left[t^2_{n+2k} + t^1_{n+2k}\,L^1(n+k) + L^2(n+2k)\,\varepsilon_{n+2k}\right]^{r-1}$$

$$\left[t^1_n\right]' = \left[t^2_n + t^1_{n-2k}\,L^1(n) + L^2(n)\,\varepsilon_{n-2k}\right]^{r-1}$$

$$\left[t^2_{n+2k}\right]' = \left[t^2_{n+2k}\,L^2(n+2k)\right]^{r-1}$$

$$\left[t^2_n\right]' = \left[t^2_{n-2k}\,L^2(n)\right]^{r-1}$$

where k = 2.

The same procedure has to be done if the range of interaction is larger with the only difference that the system of equations to be solved in order to determine the constants will be larger.

(c) Regular 2-d square lattice with n.n. interactions.

The procedure isanalogous to that outlined for the previous example. We start with the equation of motion for a given site n,m where n labels rows and m labels columns.

$$\varepsilon_{n,m} + t^1\left(n+1,m + n-1,m + n,m+1 + n,m-1\right) = 0 \ .$$

Next we write down the equations for the 4 nearest neighbours. As we want to eliminate these sites (which are "odd" sites) we multiply each of the equations by $-t^1/\varepsilon$ and sum them all. We get:

$$\left[\varepsilon - \frac{4(t^1)^2}{\varepsilon}\right]_{n,m} + \left[-\frac{2(t^1)^2}{\varepsilon}\right]\left(n+1,m+1 + n-1,m-1 + n-1,m+1 + n-1,m-1\right)$$

$$+ \left[-\frac{(t^1)^2}{\varepsilon}\right]\left(n+2,m + n-2,m + n,m+2 + n,m-2\right) = 0 \ .$$

We see that we are left with a new square lattice with $a' = \sqrt{2}\,a$ shifted by 45° with respect to the original one. As is well known, in 2-d , we have generated a new coupling upon decimation. Of course, the procedure continues to be exact. We can re-label the parameters:

$$\varepsilon_1\, n,m + t^1_1\left(n+1,m+1 + n+1,m-1 + n-1,m+1 + n-1,m-1\right) +$$

$$+ t^2_1\left(n+2,m + n-2,m + n,m+2 + n,m-2\right) = 0 \ ,$$

where the subscript indicates the order of iteration but the sites still correspond to the original lattice.

We again write down the equations (at stage 1) for the sites connected by interactions to n,m in the above equation (8 equations). We then observe that the "odd sites" to be eliminated are the nearest-neighbours to n,m on the lattice corresponding to $a' = \sqrt{2}\,a$ so we multiply their equations by $-t^1_1/\varepsilon_1$ and the rest by t^2_1/ε_1 . We sum up all the 9 equations. We observe that all the "odd sites" are cancelled out and we are left with the square lattice of $a' = 2a$ and in the same position as the original lattice (shifted back 45°). The useful observation is that all the terms where we have crossed terms (products of $t^i t^j$

with $i \neq j$) are cancelled out and all the terms which are squares of the same interaction remain. We are left with:

$$\left[\varepsilon_1 - \frac{4(t_1^1)^2}{\varepsilon_1} + \frac{4(t_1^2)^2}{\varepsilon_1}\right] n,m +$$
$$+ \left[2t_1^2 - \frac{2(t_1^1)^2}{\varepsilon_1}\right](n+2,m + n-2,m + n,m+2 + n,m-2)$$
$$+ \left[-\frac{(t_1^1)^2}{\varepsilon_1} + \frac{2(t_1^2)^2}{\varepsilon_1}\right](n+2,m+2 + n+2,m-2 + n-2,m+2 + n-2,m-2)$$
$$+ \left[\frac{(t_1^2)^2}{\varepsilon_1}\right](n+4,m + n-4,m + n,m+4 + n,m-4) = 0 \quad .$$

We next re-label the sites reducing the spacing to a for commodity only:

$$\varepsilon_2\, n,m + t_2^1(n+1,m+n-1,m+n,m+1+n,m-1) +$$
$$+ t_2^2(n+1,m+1+n+1,m-1+n-1,m+1+n-1,m-1) +$$
$$+ t_2^3(n+2,m+n-2,m+n,m+2+n,m-2) = 0 \quad .$$

We again write down the equations for all the sites connected by interactions with n,m and multiply by the adequate constants in order to eliminate the "odd sites". As we have mentioned earlier, it is sufficient to write down the squared terms only. We are left with:

$$\left[\varepsilon_2 - \frac{4(t_2^1)^2}{\varepsilon_2} + \frac{4(t_2^2)^2}{\varepsilon_2} - \frac{4(t_2^3)^2}{\varepsilon_2}\right] n,m +$$
$$+ \left[2t_2^2 - \frac{2(t_2^1)^2}{\varepsilon_2}\right](n+1,m+1+n+1,m-1+n-1,m+1+n-1,m-1)$$
$$+ \left[\frac{(t_2^2)^2}{\varepsilon_2} - \frac{2(t_2^3)^2}{\varepsilon_2}\right](n+2,m+2+n+2,m+2+n-2,m+2+n-2,m-2)$$
$$+ \left[-\frac{(t_2^3)^2}{\varepsilon_2}\right](n+4,m+n-4,m+n,m+4+n,m-4) = 0 \quad .$$

We again are left with a lattice shifted by 45^0 and of spacing $a' = 2^{3/2}a$. Notice that the new coupling that has appeared here is not between third nearest neighbours but between fourth neighbours on that lattice.

We can perform the same procedure again and again. (It is sufficient to write down the squared terms because the others get completely eliminated). However, we observe a regularity within the renormalizations of the parameters so we can generalize the obtained relations up to any order of iteration procedure:

$$[\varepsilon]^r = \left[\varepsilon + \sum_{i=1}^{r} \frac{(t^i)^2}{\varepsilon}(-1)^i\right]^{r-1}$$

$$[t^1]^r = \left[2t^2 - 2\frac{(t^1)^2}{\varepsilon}\right]^{r-1}$$

$$[t^2]^r = \left[-\frac{(t^1)^2}{\varepsilon} + 2\frac{(t^2)^2}{\varepsilon}\right]^{r-1}$$

$$[t^3]^r = \left[2t^4 + \frac{(t^2)^2}{\varepsilon} - 2\frac{(t^3)^2}{\varepsilon}\right]^{r-1} .$$

For $1 > i > r$ and i even:

$$[t^i]^r = \left[-\frac{(t^{i-1})^2}{\varepsilon} + 2\frac{(t^i)^2}{\varepsilon}\right]^{r-1} .$$

For $1 > i > r$ and i odd:

$$[t^i]^r = \left[\frac{(t^{i-1})^2}{\varepsilon} - 2\frac{(t^i)^2}{\varepsilon} + 2t^{i+1}\right]^{r-1} .$$

For $i = r$

$$[t^r]^r = \left[-\frac{(t^{r-1})^2}{\varepsilon} + 2\frac{(t^r)^2}{\varepsilon}\right](-1)^r .$$

For $i = r+1$

$$[t^{r+1}]^r = \left[(-1)^r\frac{(t^r)^2}{\varepsilon}\right] .$$

So the decimation on the regular square lattice in 2-d can be carried out automatically up to any stage with ease. The above described procedure is that outlined by Southern et al. [14] but they study a finite size lattice (8 x 8 in 2-d). The procedure can, in principle, be applied in the same way to the disordered 2-d lattice but the algebra is much more cumbersome.

III. FINAL COMMENTS

Once the decimation procedure has been performed it is necessary to know how to extract physical information from the renormalized problem. We have

discussed one possible procedure [9),15)] for 1-d problems. We want to apply the same criterion for the square lattice but the numerical evaluation of this part has not been completed yet. However, we have confidence of getting good results because Southern et al. [14)] get quite good numbers already for a finite size system. Namely the idea is to see the convergence of the different hopping coefficients with iteration at different values of energy and then to extract the density of states from the diagonal renomalized parameter as explained in Refs.9) and 15). Another point is to establish how quick convergence actually is and decide how many interactions are relevant for a good answer. This is necessary information if one wants to process a disordered 2-d problem in a reasonably approximated way because there, due to the number of equations involved at more advanced iterations, it is very difficult to get a general formula as in the pure case.

We also think that the 1-d problem with disordered 1^{st} and 2^{nd} neighbours interactions is also worth studying in the same way.

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