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Hubbard model: revisited—a macroscopic renormalization group study

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Abstract. The spin-correlation length is used to set up a RG analysis of the Hubbard model (within RPA). We demonstrate that an identical critical behaviour is obtained by performing the macroscopic renormalization group analysis with the antisymmetric Landau interaction parameter. The beta functions for the half-filled and quarter-filled band cases have been evaluated.

Keywords. Hubbard model; macroscopic renormalization group; beta function.

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1. Introduction

In this paper we have taken the RPA (random phase approximation) solution to the Hubbard model as a toy model of a system with short-ranged interaction and demonstrated that the Landau interaction parameter is, indeed, the appropriate physical property of this system to be used with the macroscopic renormalization group (MRG) method. This method was applied recently (Singh and McMillan 1985b) to the Anderson model with weak, short-ranged interactions to examine the relevance of interactions near the non-interacting fixed point. We have used the spin-correlation length to set up a RG analysis and shown that the critical behaviour can identically be obtained by performing the MRG with the antisymmetric Landau interaction parameter.

The MRG method, applied initially to study classical spin systems, (McMillan 1984) has proved to be equally convenient for some quantum systems such as the Anderson model (Singh and McMillan 1985a) and the case with interactions (Singh 1987). The basic idea behind the MRG method is to compute certain macroscopic physical quantities for finite lattice systems with different lattice parameters and as a function of the Hamiltonian parameters, and then require that the physical properties be preserved with respect to changes in the lattice parameter. This generates, implicitly, a recursion relation between the Hamiltonian parameters from which one can study the critical behaviour.

The correct choice of physical properties is essential. Relevant, scaling variables (e.g. conductance in the problem of an electron moving in a random potential) will always be appropriate. Otherwise, in case of doubt, one can always use the appropriate correlation length. In classical spin systems it is well-known that the width of the soliton-like domain wall which describes the magnetization domain boundary is related to the spin-correlation length in the system. And since the domain-wall energy depends upon the width and hence on the correlation length, it is an appropriate MRG variable. For the Hubbard model studied here we similarly show that the antisymmetric Landau parameter involves the same effective interaction as the spin-correlation length (within RPA).

The MRG offers certain advantages, especially in quantum systems, over conventional real-space RG methods. The Migdal-Kadanoff decimation procedure, for example, which is so convenient and simple when applied to classical spin-systems is, however, beset with problems due to the non-commutating nature of pieces in the Hamiltonian for a typical quantum system (Suzuki and Takano 1979). The block method has problems of its own (Ma 1982) when dealing with a disordered system.

2. Macroscopic renormalization group

To illustrate the essential features of the MRG technique for an interacting system we have applied it to the $1d$ Hubbard model within RPA for the half-filled and quarter-filled band cases. The Hamiltonian we study is,

$$H=\sum_{\sigma,\langle ij\rangle} V(a_{i\sigma}^{\dagger}a_{j\sigma}+a_{j\sigma}^{\dagger}a_{i\sigma})+U\sum_{i} a_{i\uparrow}^{\dagger}a_{i\uparrow}a_{i\downarrow}^{\dagger}a_{i\downarrow}. \tag{1}$$

The RG is generated implicitly by matching the spin-correlation length, ξ.

$$\xi_{n'}(U')/L'=\xi_{n}(U)/L, \tag{2}$$

where $L=na=n'a'=L'$ is the physical length of the two lattice systems; a and a' are the lattice parameters and n and n' are the number of sites in the two systems.

The spin-correlation function, $S(\mathbf{q},\omega)\equiv\int dt\exp(i\omega t)\langle\sigma^{-}(\mathbf{q},t)\sigma^{+}(-\mathbf{q},0)\rangle$ in RPA is related to the static susceptibility via the fluctuation-dissipation theorem and the Kramers-Kronig relation (see e.g. Blandin (1976)). For $(1-UN(0)qv_F\ll kT$, it is found to be given by: $S(q,\omega)=\pi kT\chi(q,0)\delta(\omega)$. After the frequency integral we then see that the static correlation function, $S(q,t=0)$ is related to the static susceptibility. To obtain the spin-correlation length we therefore look at the static magnetic susceptibility in the RPA obtained via the Kubo formula (Doniach and Sondheimer 1974) and compare it with the Ornstein-Zernike form (Fisher 1982)

$$\chi_{ij}^{-+}=[\mathbf{I}/(1-U\mathbf{I})]_{ij}, \tag{3}$$

$$(\mathbf{I})_{ij}=i\int\frac{d\omega}{2\pi}G_{ij}^{\uparrow}(\omega)G_{ij}^{\downarrow}(\omega), \tag{4}$$

$(\mathbf{I})_{ij}$ is the susceptibility matrix for the non-interacting system. i, j refer to sites in the lattice system. In the paramagnetic phase the Green's functions are spin-independent. Since we are interested in $T\ll T_F$, we evaluate $\mathbf{I}$ at $T=0$ and ignore the $O(T/T_F)$

corrections. In terms of the eigenfunctions, $\{|\phi_l\rangle\}$ and eigenvalues, $\{\varepsilon_l\}$ of the non-interacting Hamiltonian for a lattice system with n sites, we obtain,

$$(\mathbf{I}_n)_{ij} = 2 \sum_{\substack{\varepsilon_l(>\varepsilon_F) \\ \varepsilon_m(<\varepsilon_F)}} \frac{\phi_l^i \phi_l^j \phi_m^i \phi_m^j}{\varepsilon_l - \varepsilon_m}. \tag{5}$$

At zero temperature the Fermi-energy is determined simply by counting states. For a system with n sites and a filling fraction f, the lower nf states are occupied. Since the eigen-energies are in ascending order with respect to their labels, the Fermi-energy lies just above $\varepsilon_{(nf)}$. $(\mathbf{I}_n)_{ij}$ depends only on the separation $|i-j|$ and exhibits the RKKY oscillation with decreasing amplitude and a period equal to twice the lattice spacing for the half-filled band case and four times the lattice spacing for the quarter-filled band case. It is this feature of the non-interacting susceptibility which leads to a magnetic ordering with oscillating magnetization in the interacting system. Fourier transformation leads to

$$I_n(Q) = \sum_{\frac{r}{a}=0}^{n-1} \cos(Qr)(\mathbf{I}_n)_{\frac{r}{a}=|i-j|}, \tag{6}$$

$$\chi_n^{-+}(Q) = \frac{I_n(Q)}{1 - UI_n(Q)}. \tag{7}$$

For the half-filled and quarter-filled band cases $I_n(Q)$ is sharply peaked at $Q=\pi/a$ and $Q=\pi/2a$ respectively, indicating that with increasing U the systems exhibit antiferromagnetic instabilities with periods of $2a$ and $4a$ respectively. If we let q indicate the deviation in Q from π/a and $\pi/2a$ for the half-filled and quarter-filled band cases respectively, then, in the limit of long wavelength $(qL \ll 1)$ we have from (6)

$$I_n(q) = \sum_{\frac{r}{a}=0}^{n-1} \cos(2f\pi r/a)(1 - \tfrac{1}{2}q^2r^2)(\mathbf{I}_n)_{\frac{r}{a}=|i-j|} \tag{8}$$

$$\equiv A_n - B_n q^2. \tag{9}$$

Substituting this in (7) for the transverse magnetic susceptibility we obtain,

$$\chi_n^{-+}(q) = \frac{A_n - B_n q^2}{UB_n\{q^2 + (1 - UA_n)/UB_n\}}. \tag{10}$$

The transition point is given by $1 - U^*A_n = 0$ and in the limit of infinite number of lattice points one gets the correct result $U^* = 0$. The small U in the denominator is, however, not a problem because if one does the analysis for an infinite system one finds that $(1 - UA)/UB$ is actually vanishing. Comparing (10) (which expresses the spatial correlation of spin-density fluctuations) with the Ornstein-Zernike form, we obtain the spin-correlation length, ξ.

$$\xi_n = a\left(\frac{UB_n}{1 - UA_n}\right)^{1/2}. \tag{11}$$

The MRG scheme (equation (2)) then leads to,

$$\frac{1}{n'}\left(\frac{U'B_{n'}}{1-U'A_{n'}}\right)^{1/2}=\frac{1}{n}\left(\frac{UB_n}{1-UA_n}\right)^{1/2}. \tag{12}$$

3. Results

Using the eigenfunctions and eigenvalues of the non-interacting Hamiltonian matrix with periodic boundary conditions, obtained numerically, we evaluate A_n and B_n for several values of n. The results are plotted in figure 1. A_n goes as the log of n and B_n as the square of n in both cases ($f=1/2$ and 1/4). Substituting the n^2 dependence of B_n (which is expected from dimensional analysis) in (12) we obtain a very suggestive form of the RG equation:

$$U'/(1-U'A_{n'})=U(1-UA_n). \tag{13}$$

As shown in §4 it turns out that $U/(1-UA_n)$ is nothing but the effective interaction which appears in the antisymmetric Landau parameter (within the same approximation).

The transition point is given by $1-UA_n=0$, and as A_n grows to ∞ logarithmically with n, we have $U^*=0$. From the recursion relation in (13) it is evident that $U^*=0$ is also the fixed point. If we express $A_n=k_A\ln n$, then for $n'=n/2$, we get

$$U'=\frac{U}{1-Uk_A\ln 2}. \tag{14}$$

Expanding around the fixed point $U^*=0$, we have

$$U'-U=U^2k_A\ln 2, \tag{15}$$

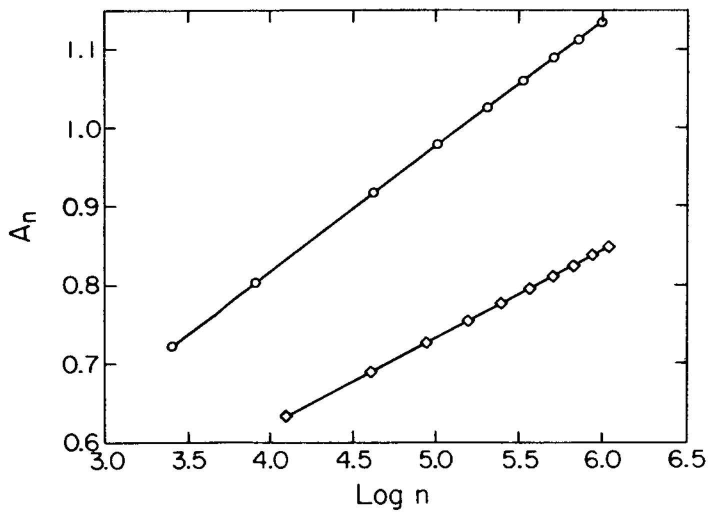

Figure 1. Plot of A_n vs $\log n$ for half-filled (circles) and quarter-filled (diamonds) band cases, $(30\leqslant n\leqslant 420)$.

from which we obtain the beta function,

$$\beta(U)=\frac{\Delta U}{\Delta \ln n}\bigg|_{\xi}=k_A U^2=0{\cdot}1591U^2 \quad (f=1/2)$$

$$=0{\cdot}1109U^2 \quad (f=1/4), \tag{16}$$

which indicates that the fixed point is marginally relevant. For comparison the result obtained analytically for the half-filled band case (see Appendix) is:

$$\beta=\frac{1}{2\pi}U^2=0{\cdot}1591U^2. \tag{17}$$

4. Landau interaction parameter

As shown in § 3 the quantity $U/(1-UI(2f\pi))$ in (13) plays an important role in the RG analysis done with spin-correlation length (within RPA). We shall now show that within the same approximation scheme, this quantity is nothing but the effective interaction which appears in the antisymmetric Landau parameter.

As was shown recently (Singh and Fradkin 1987) the ladder diagrams leading to the RPA magnetic susceptibility (Doniach and Sondheimer 1974) are of order 1 within a $1/N$ expansion type perturbation theoretic treatment of the corresponding N-orbital model. To $O(1)$ then, we evaluate the interaction energies between quasiparticles. There are two sets of bubble diagrams, with even and odd number of bubbles, which

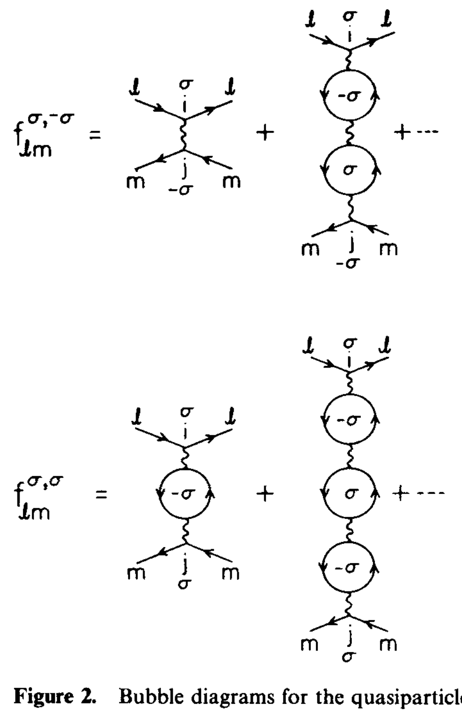

Figure 2. Bubble diagrams for the quasiparticle interaction energies.

contribute to the interaction energies $f_{lm}^{\sigma,-\sigma}$ and $f_{lm}^{\sigma,\sigma}$, respectively (figure 2). Here l and m refer to the quasiparticle states. In terms of the effective interaction strengths, $U_{\rm eff}^{\sigma,\sigma'}(i,j)$ between quasiparticles at sites i and j, we can write down the interaction energies as:

$$f_{lm}^{\sigma,\sigma'} = \sum_{i,\, j\geq i} (\phi_l^i)^2(\phi_m^j)^2 U_{eff}^{\sigma,\sigma'}(i,j) \tag{18}$$

where

$$U_{\rm eff}^{\sigma,-\sigma}(i,j) = \left(\frac{U}{\mathbf{1}-U^2\mathbf{I}^2}\right)_{ij}, \tag{19}$$

and

$$U_{\rm eff}^{\sigma,\sigma}(i,j) = -\left(\frac{U^2\mathbf{I}}{\mathbf{1}-U^2\mathbf{I}^2}\right)_{ij}, \tag{20}$$

where $(\mathbf{I})_{ij}$ is the bubble term defined in (4). The antisymmetric part is given by,

$$\begin{aligned} f_{lm}^a &= f_{lm}^{\sigma,\sigma} - f_{lm}^{\sigma,-\sigma} \\ &= -\sum_{i,\,j}\left(\frac{U}{\mathbf{1}-U\mathbf{I}}\right)_{ij}(\phi_l^i)^2(\phi_m^j)^2. \end{aligned} \tag{21}$$

Let us consider the half-filled band case for concreteness. The antiferromagnetic instability will correspond, in this formulation of interaction energies, to the first singularity in the matrix $U/(\mathbf{1}-U\mathbf{I})$ with increasing U. This occurs when the largest eigenvalue, $\lambda_{\rm max}$ of the polarization bubble matrix, $\mathbf{I}$ equals $1/U$. The eigenvector of $\mathbf{I}$ corresponding to this largest eigenvalue consists of elements which are all equal in magnitude and alternating in sign. And therefore, in view of the alternating signs of $(\mathbf{I})_{ij}$, we have

$$\begin{aligned} \lambda_{\rm max} &= \sum_j |(\mathbf{I})_{ij}| \\ &= \sum_{\frac{r}{a}=0} \cos(\pi r/a)(\mathbf{I})_{\frac{r}{a}=|i-j|} \\ &= A, \end{aligned} \tag{22}$$

where A has been defined in (8). The interaction energy corresponding to the antiferromagnetic mode is thus obtained from (21):

$$f_{lm}^a(\pi) = -\sum_i (\phi_l^i)^2(\phi_m^i)^2\left(\frac{U}{1-UA}\right). \tag{23}$$

The Landau parameter is finally obtained by taking $l=m$ and multiplying by the density of states at the Fermi-energy.

$$F^a = -N(0)\sum(\phi_l^i)^4\left(\frac{U}{1-UA}\right). \tag{24}$$

The MRG is now defined by requiring that the antisymmetric Landau parameter be preserved as one varies the lattice parameter.

$$F^a_{n'}(U') = F^a_n(U). \tag{25}$$

Since the density of states, $N(0)$ is proportional to n and the wavefunctions are proportional to $1/n^{1/2}$, we see that the RG relation in (25) reduces to:

$$\frac{U'}{1-U'A'_{n'}} = \frac{U}{1-UA_n}, \tag{26}$$

which is precisely the recursion relation obtained in § 3 starting with the spin-correlation length.

5. Conclusion

In this paper we have taken the RPA result for the spin-correlation length in a system with short-ranged interaction to set up a macroscopic renormalization group. We have shown that use of the antisymmetric Landau parameter within the same approximation scheme generates an identical recursion relation. We have applied the RG method to the $1d$ system, in particular, with half-filled and quarter-filled bands and have evaluated the beta functions. For the half-filled band case the coefficient of the U^2 term in $\beta(U)$ agrees excellently with the analytical result of $1/2\pi$ obtained within RPA.

In the MRG method one approaches the paramagnetic-antiferromagnetic transition from the paramagnetic side, whereas in the analytical treatment one must consider the finite gap in the energy bands in evaluating the Green's functions in the antiferromagnetic phase. This aspect makes the numerical MRG method exceedingly more convenient and versatile for studying systems with arbitrary band-filling. The method suggests how to go beyond first order in interaction strength when using the Landau parameter to study disordered, interacting systems by incorporating the magnetic ordering resulting from spin fluctuations. In addition, a formulation in terms of the Landau parameter may be more apt for systems like the $2d$ itinerant model with parabolic band which is not yet fully understood (Theumann and Béal-Monod 1984). In this system the susceptibility of the non-interacting system is constant for $0 \leqslant q \leqslant k_F$ and so $\Sigma_{q=0}^{k_F} F^a(q)$ should be the appropriate quantity to use.

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Appendix

Here we sketch out briefly the evaluation of the beta function for the half-filled band case. In a $1d$ lattice system the antiferromagnetic instability occurs at $U=0$ and for a finite value of U the energy band has a gap, 2Δ. Δ is obtained (within RPA) by solving self-consistently the equation for spin-densities and is given (in the limit $\Delta \ll 1$) by:

$$\Delta = 2\exp(-2\pi/U). \tag{A1}$$

(The energies, U and Δ are measured relative to the hopping strength, V). Incorporating the proper spin-dependence of quasiparticle energies in the Green's functions, we evaluate

$$I(Q, U) = i \int \frac{d\omega}{2\pi} \int_{-\pi}^{\pi} \frac{dk}{2\pi} G^{\uparrow}(k, \omega; U) G^{\downarrow}(k - Q, \omega; U). \tag{A2}$$

Expanding around $Q = \pi$, we find for small q,

$$I(q, U) = \frac{3}{4U} - \frac{1}{4\pi\Delta^2} q^2. \tag{A3}$$

From equation (3) we obtain the transverse magnetic susceptibility and the spin-correlation length:

$$\xi(U) = \frac{1}{\Delta}\left(\frac{U}{\pi}\right)^{1/2}$$

$$= \frac{1}{2}\left(\frac{U}{\pi}\right)^{1/2} \exp(2\pi/U). \tag{A4}$$

The beta function is then found as,

$$\beta(U) = -1 \Big/ \frac{d}{dU} \ln\left\{\frac{1}{2}\left(\frac{U}{\pi}\right)^{1/2} \exp(2\pi/U)\right\}$$

$$= \frac{U^2}{2\pi} \quad (\text{as } U \to 0). \tag{A5}$$

The fixed point ($\beta(U^*) = 0$) is thus at $U = 0$ and it is marginally relevant in nature.

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