Vol. 34 (2003) *ACTA PHYSICA POLONICA B* No 2

A STRONG EFFECT OF DISORDER ON MOTT TRANSITION: HUBBARD-LLOYD MODEL*

J. Spałek
Marian Smoluchowski Institute of Physics, Jagellonian University
Reymonta 4, 30-059 Kraków, Poland

and W. Wójcik
Institute of Physics, Tadeusz Kościuszko Technical University
Podchorążych 1, 30-084 Kraków, Poland

(Received July 10, 2002)

We include atomic disorder in correlated narrow-band systems by assuming that the atomic level position fluctuates according to the Lorentzian distribution. We use the *Lloyd exact form* of the averaged single-particle Green function when the electronic correlations are absent or treated in the saddle-point slave-boson (or Gutzwiller) approximation. The weak disorder reduces *drastically* the threshold for the Mott–Hubbard localization.

PACS numbers: 71.27.+a, 71.30.+h, 71.23.–k

The effect of atomic and thermal disorder on electronic properties of correlated electronic systems is of great interest, particularly close to a quantum critical point, where a non-Fermi liquid behavior or the Mott–Hubbard localization are observed. The disorder is so influential in the critical regime because the system is at a threshold of an instability and therefore, a weak perturbation produces a disproportionate effect by changing the nature of the quantum macro state.

We propose a *physical model*, which allows for a simple (and partly exact) analysis of the atomic-disorder role on the physical properties of almost localized systems. Namely, we consider first the mean-field (saddle-point Gutzwiller) picture of quasiparticle states and then determine the drastic influence on them of a weak disorder treated exactly.

We start with a half-filled narrow-band system of correlated electrons characterized by the quasiparticle energies $E_{\boldsymbol{k}} = q\varepsilon_{\boldsymbol{k}}$, where $\varepsilon_{\boldsymbol{k}}$ is the bare band energy and q is the band narrowing factor [1]. Explicitly, for a half-filled band configuration ($n = 1$) $q = 8d^2(1 - 2d^2)$, where d^2 is the probability of

---

[*] Presented at the International Conference on Strongly Correlated Electron Systems, (SCES 02), Cracow, Poland, July 10–13, 2002.

having a double occupancy on a single atomic site. We introduce the atomic disorder in the system by assuming that the atomic level position fluctuates around the mean value $\varepsilon_0 = 0$. In result, the starting effective Hamiltonian for N sites in real space takes the form

$$H = \sum_{i\sigma} \varepsilon_i n_{i\sigma} + q \sum_{ij\sigma}{}' t_{ij} a_{i\sigma}^{\dagger} a_{j\sigma} + U d^2 N \,, \tag{1}$$

where t_{ij} is the hopping integral and U is the magnitude of intraatomic interaction i. In this manner, we assume that the disorder is weak and therefore, the mean-field-like quasiparticle states with energies $q\varepsilon_{\boldsymbol{k}}$ are formed first [2]. Furthermore, we assume that the disorder is represented by the Lorentzian distribution of the atomic-level portion $\varepsilon = \{\varepsilon_i\}$, *i.e.*

$$P(\varepsilon) = \frac{\varepsilon_1}{\pi} \frac{1}{(\varepsilon - \varepsilon_0)^2 + \varepsilon_1^2} \,, \tag{2}$$

where ε_1 is the distribution width. Under these circumstances, the Hamiltonian (1) is **exactly soluble** and the expression for the single-particle Green function takes a very simple form [3]

$$G_{\boldsymbol{k}}(E) = \frac{1}{E - q\varepsilon_{\boldsymbol{k}} - \bar{\varepsilon} + i\varepsilon_1} \equiv \frac{1}{E - (\varepsilon_{\boldsymbol{k}} - \mu) - \Sigma} \,, \tag{3}$$

where $\bar{\varepsilon} = \varepsilon_0 + \mu$, and μ is the chemical potential. The disorder introduces the quasiparticle lifetime $\hbar/\varepsilon_1$, whereas the correlations renormalize the particle mass $m_0 \to m^* \equiv m_0/q$ [1]. This is because the selfenergy in (3) is $\Sigma(E) = -(1-q)E - i\varepsilon_1$. The spectral density function $A_{\boldsymbol{k}}(E)$ is then given by

$$A_{\boldsymbol{k}}(E) \equiv -\frac{1}{\pi} \mathrm{Im} G_{\boldsymbol{k}}(E) = \frac{1}{\pi} \frac{\varepsilon_1}{(E - \bar{\varepsilon} - q\varepsilon_{\boldsymbol{k}})^2 + \varepsilon_1^2} \,. \tag{4}$$

Thus, the spectral density function is also of Lorentzian form. The density of states (per one spin direction) for this system is, in turn, determined from the relation

$$\rho(E) = \frac{\varepsilon_1}{\pi} \int\limits_{-W/2}^{W/2} d\varepsilon \frac{\rho_0(\varepsilon)}{(E - \bar{\varepsilon} - q\varepsilon)^2 + \varepsilon_1^2} \,, \tag{5}$$

where $\rho_0(\varepsilon)$ is the density of states in the bare band. For the modeling purposes, we take a constant density of states ($\rho_0(\varepsilon) = 1/W$, for $-W/2 \leq \varepsilon \leq W/2$), as Eq. (5) involves an integration and thus should not depend much on the detailed band shape (within a numerical factor). In result, the density of states at the Fermi level ($E = \bar{\varepsilon} = 0$) is

$$\rho(0) = \frac{2}{\pi q W} \arctan\left(\frac{Wq}{2\varepsilon_1}\right) \simeq \frac{2}{\pi q W} \begin{cases} \frac{qW}{\varepsilon_1} & \text{for } \frac{qW}{2\varepsilon_1} \ll 1 \\ \frac{\pi}{2} - \frac{2\varepsilon_1}{qW} & \text{for } \frac{qW}{2\varepsilon_1} \gg 1\,. \end{cases} \tag{6}$$

The upper limiting situation corresponds to the strong-disorder case, whereas the lower will represent the weak-disorder limit.

Taking the density of states (6) we can calculate the ground state energy E_{G}. Using the condition $\partial E_{\mathrm{G}}/\partial q = 0$, we obtain the equation for q (or d^2) in the closed form:

$$\left[\frac{2\varepsilon_1}{W} - q \arctan\left(\frac{qW}{2\varepsilon_1}\right)\right] \sqrt{1-q} + \frac{U}{U_{\mathrm{c}}} \frac{qW}{2} = 0\,, \tag{7}$$

where $U_{\mathrm{c}} = 2W$ is the localization threshold when the disorder is absent.

The explicit form (4) of the spectral density function allows us also to calculate statistical distribution function at $T = 0$, which is

$$\bar{n}_{\boldsymbol{k}\sigma} = \int\limits_{-\infty}^{\mu} dE A_{\boldsymbol{k}}(E) = \frac{1}{2} - \frac{1}{\pi} \arctan\left(\frac{q\varepsilon_{\boldsymbol{k}} - \mu}{\varepsilon_1}\right)\,. \tag{8}$$

This is a general formula, with the band shape $\varepsilon_{\boldsymbol{k}}$. Only in the case $\varepsilon_1 = 0$ do we recover the Fermi–Dirac distribution $\bar{n}_{\boldsymbol{k}\sigma} = \Theta(\mu - q\varepsilon_{\boldsymbol{k}})$. Therefore, in this respect our system is certainly a *non-Landau (non-Fermi) liquid*, as the $\mathrm{Im}\Sigma(E)$ does not vanish for $E = \mu$ and thus for $E_{\boldsymbol{k}} \to \mu$, $q|\varepsilon_{\boldsymbol{k}}| \ll \varepsilon_1$, even though $\varepsilon_1/W \ll 1$.

To illustrate our results, we have plotted in Fig. 1 the localization threshold (for which $d^2 = 0$), which is strongly reduced for relatively small value

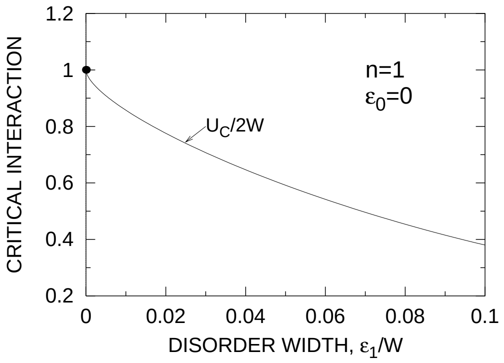

Fig. 1. Critical interaction U/U_{c} for the localization threshold *vs* ε_1/W.

of ε_1/W. The density of states determines directly the electronic specific heat coefficient γ. The static paramagnetic susceptibility $\chi(0)$ has the form provided earlier [4]. Therefore, one can determine the dimensionless value of the *Wilson ratio* $R = (\chi/\chi_0)/(\gamma/\gamma_0)$, where γ_0 and χ_0 are the values for the uncorrelated pure systems.

In Fig. 2 we have plotted this ratio as a function of the relative interaction strength. In the pure system ($\varepsilon_1 = 0$) the ratio evolves from unity at $U = 0$ to the value $R = 4$ at $U = U_c$ [4]. The disorder washes out systematically that dependence and makes the system look like less correlated, *even though the density of states is strongly enhanced.*

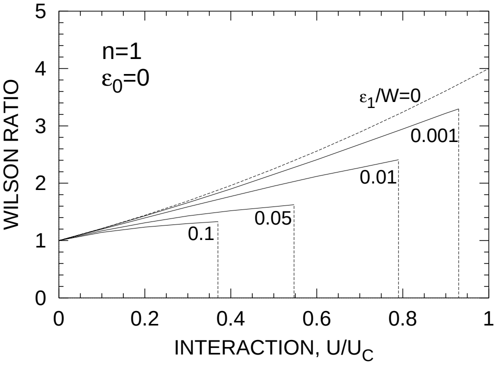

Fig. 2. The Wilson parameter *vs* U/U_c for several values of ε_1/W.

In summary, we have devised a simple physical model describing a non-Fermi liquid behavior induced by the atomic disorder in almost localized systems. A weak disorder sharply reduces the localization threshold and the Wilson ratio in the correlated state.

The work was supported by the Polish State Committee for Scientific Research (KBN), Grant No. 2 P03B 050 23.

REFERENCES

[1] J. Spałek, A. Datta, J.M. Honig, *Phys. Rev. Lett.* **59**, 728 (1987); J. Spałek, W. Wójcik, in *Spectroscopy of Mott Insulators and Correlated Metals*, Springer, Berlin 1995, pp.41-65.

[2] In this manner, we neglect the correlation effects between the atomic disorder and the quantum fluctuations.

[3] P. Lloyd, *J. Phys.* **C2**, 1717 (1969); M. Acquarone, D.K. Ray, J. Spałek, *J. Phys.* **C15**, 959 (1982).

[4] J. Spałek, *J. Solid State Chem.* **88**, 70 (1990).