An important equation for the Anderson model

1995 J. Phys.: Condens. Matter 7 867

(http://iopscience.iop.org/0953-8984/7/5/008)

J. Phys.: Condens. Matter 7 (1995) 867–871. Printed in the UK

An important equation for the Anderson model

Baohua Teng

Department of Physics, Chengdu University of Science and Technology, Chengdu, Sichuan 610065, People's Republic of China

Received 26 August 1994, in final form 19 October 1994

Abstract. This paper proves an important equation for the Anderson model. Then, using this equation we deal exactly with the Anderson model and obtain the exact analytical expression for the ground-state energy. This result coincides with the result of the Bethe *ansatz*.

1. Introduction

The Anderson [1] model is an important topic in condensed-matter physics. It has been dealt with by many approximate methods [2–4]. Although Andrei [5] and Wiegmann [6] solved the Anderson model exactly within the framework of the Bethe *ansatz*, they cannot give exact analytical expressions for the physical quantities concerned with the model.

This paper deals with two features. First, we have proved an important equation for the Anderson model. Then, using this equation, we exactly solve the Anderson Hamiltonian and obtain the exact analytical expression for the ground-state energy of the model.

2. An important equation

The single-impurity Anderson [1] model, in the standard notation is

$$H = \sum_{k,\sigma}(\varepsilon_k - \varepsilon_f)a^+_{k\sigma}a_{k\sigma} + \sum_{\sigma}(\varepsilon_d - \varepsilon_f)c^+_{d\sigma}c_{d\sigma} + Un_{d\sigma}n_{d-\sigma} + \sum_{k,\sigma}(V_{kd}a^+_{k\sigma}c_{d\sigma} + \mathrm{HC}). \tag{1}$$

According to the Green function technique used by Zubarev [7], we define the Green functions as follows:

$$G^{(1)}_{dd,\sigma}(\omega+\varepsilon_f) \equiv \langle\langle c_{d\sigma}; c^+_{d\sigma}\rangle\rangle(\omega) \qquad G^{(2)}_{kd,\sigma}(\omega+\varepsilon_f) \equiv \langle\langle a_{k\sigma}; c^+_{d\sigma}\rangle\rangle(\omega)$$

$$G^{(3)}_{kk,\sigma}(\omega+\varepsilon_f) \equiv \langle\langle a_{k\sigma}; a^+_{k\sigma}\rangle\rangle(\omega) \qquad \Gamma^{(1)}_{dd,\sigma}(\omega+\varepsilon_f) \equiv \langle\langle n_{d-\sigma}c_{d\sigma}; c^+_{d\sigma}\rangle\rangle(\omega)$$

$$\Gamma^{(2)}_{dk,\sigma}(\omega+\varepsilon_f) \equiv \langle\langle n_{d-\sigma}c_{d\sigma}; a^+_{k\sigma}\rangle\rangle(\omega) \qquad F_{dd,\sigma}(\omega+\varepsilon_f) \equiv \langle\langle n_{d-\sigma}c_{d\sigma}; n_{d-\sigma}c^+_{d\sigma}\rangle\rangle(\omega).$$

So we have the equations of motion given by

$$(\omega - \varepsilon_d)G^{(1)}_{dd,\sigma}(\omega) = 1 + U\Gamma^{(1)}_{dd,\sigma}(\omega) + \sum_k V_{kd}G^{(2)}_{kd,\sigma}(\omega) \tag{2}$$

$$(\omega - \varepsilon_k)G^{(2)}_{kd,\sigma}(\omega) = V_{kd}G^{(1)}_{dd,\sigma}(\omega) \tag{3}$$

$$(\omega-\varepsilon_k)G^{(3)}_{kk,\sigma}(\omega)=1+V_{kd}G^{(2)}_{kd,\sigma}(\omega) \tag{4}$$

$$(\omega-\varepsilon_d)\Gamma^{(1)}_{dd,\sigma}(\omega)=\langle n_{d-\sigma}\rangle+UF_{dd,\sigma}(\omega)+\sum_k V_{kd}\Gamma^{(2)}_{dk,\sigma}(\omega) \tag{5}$$

$$(\omega-\varepsilon_k)\Gamma^{(2)}_{dk,\sigma}(\omega)=V_{kd}\Gamma^{(1)}_{dd,\sigma}(\omega) \tag{6}$$

and the equation of ensemble average given by

$$\begin{aligned}\langle n_{d-\sigma}n_{d\sigma}\rangle &= -\frac{1}{\pi}\int_{-\infty}^{\infty} f(\omega-\varepsilon_f)\,\mathrm{Im}[\Gamma^{(1)}_{dd,\sigma}(\omega+\mathrm{i}0)]\,\mathrm{d}\omega\\ &= -\frac{1}{\pi}\int_{-\infty}^{\infty} f(\omega-\varepsilon_f)\,\mathrm{Im}[F_{dd,\sigma}(\omega+\mathrm{i}0)]\,\mathrm{d}\omega\end{aligned} \tag{7}$$

in the usual way [7].

Now we prove that an important equation holds, i.e. that $\Gamma^{(1)}_{dd,\sigma}(\omega)=F_{dd,\sigma}(\omega)$ for the Anderson model.

Firstly, according to equation (7), the double occupation $\langle n_{d-\sigma}n_{d\sigma}\rangle$ is decided by $-(1/\pi)\,\mathrm{Im}[\Gamma^{(1)}_{dd,\sigma}(\omega+\mathrm{i}0)]$ and $-(1/\pi)\,\mathrm{Im}[F_{dd,\sigma}(\omega+\mathrm{i}0)]$ to the same extent.

Secondly, according to the physical meaning of the Anderson model, at a certain temperature, $\langle n_{d-\sigma}n_{d\sigma}\rangle$ is continuously decreasing while U increases; thus

$$\langle n_{d-\sigma}n_{d\sigma}\rangle=\begin{cases}\langle n_{d-\sigma}\rangle\langle n_{d\sigma}\rangle & U=0\\ 0 & U\to\infty.\end{cases}$$

Therefore let $0\leqslant U_1<U_2<\cdots<U_N<\infty$; at a certain temperature we have

$$\begin{aligned}&-\frac{1}{\pi}\int_{-\infty}^{\infty} f(\omega-\varepsilon_f)\,\mathrm{Im}[\Gamma^{(1)}_{dd,\sigma}(\omega+\mathrm{i}0,U_i)]\,\mathrm{d}\omega\\ &\quad= -\frac{1}{\pi}\int_{-\infty}^{\infty} f(\omega-\varepsilon_f)\,\mathrm{Im}[F_{dd,\sigma}(\omega+\mathrm{i}0,U_i)]\,\mathrm{d}\omega\\ &\quad> -\frac{1}{\pi}\int_{-\infty}^{\infty} f(\omega-\varepsilon_f)\,\mathrm{Im}[\Gamma^{(1)}_{dd,\sigma}(\omega+\mathrm{i}0,U_j)]\,\mathrm{d}\omega\\ &\quad= -\frac{1}{\pi}\int_{-\infty}^{\infty} f(\omega-\varepsilon_f)\,\mathrm{Im}[F_{dd,\sigma}(\omega+\mathrm{i}0,U_j)]\,\mathrm{d}\omega\end{aligned}$$

where $i<j=2,3,\ldots,N$. So $-(1/\pi)\,\mathrm{Im}[\Gamma^{(1)}_{dd,\sigma}(\omega+\mathrm{i}0)]$ and $-(1/\pi)\,\mathrm{Im}[F_{dd,\sigma}(\omega+\mathrm{i}0)]$ are some peak-like distributions whose locations are related to U.

Thirdly, according to equation (7) and the well known formula

$$\int_{-\infty}^{\infty} f(\omega-\varepsilon_f)A(\omega)\,\mathrm{d}\omega=\int_{-\infty}^{\varepsilon_f}A(\omega)\,\mathrm{d}\omega+\frac{\pi^2}{6}T^2A'(\varepsilon_f)+\frac{7\pi^4}{360}T^4A'''(\varepsilon_f)+\cdots$$

we have

$$\int_{-\infty}^{\varepsilon_f}A(\omega)\,\mathrm{d}\omega=\int_{-\infty}^{\varepsilon_f}B(\omega)\,\mathrm{d}\omega \tag{8a}$$

$$A'(\varepsilon_f)=B'(\varepsilon_f) \tag{8b}$$

$$A'''(\varepsilon_f)=B'''(\varepsilon_f) \tag{8c}$$

where $A(\omega) = -(1/\pi)\,\mathrm{Im}[\Gamma^{(1)}_{dd,\sigma}(\omega + \mathrm{i}0)]$ and $B(\omega) = -(1/\pi)\,\mathrm{Im}[F_{dd,\sigma}(\omega + \mathrm{i}0)]$.

Because U is not related to ε_f and according to equations (2)–(6), neither $\Gamma^{(1)}_{dd,\sigma}(\omega)$ nor $F_{dd,\sigma}(\omega)$ is the explicit function with respect to ε_f; solving equation (8*b*) for arbitrary ε_f, and using equation (8*a*), we obtain $A(\omega) = B(\omega)$.

Finally, using

$$\mathrm{Re}[G(\omega + \mathrm{i}0)] = \frac{p}{\pi}\int_{-\infty}^{\infty} \frac{\mathrm{Im}[G(\omega' + \mathrm{i}0)]}{\omega - \omega'}\,\mathrm{d}\omega'$$

we come to the conclusion that

$$\Gamma^{(1)}_{dd,\sigma}(\omega) = F_{dd,\sigma}(\omega) \tag{9}$$

holds exactly for the Anderson model.

3. The ground-state energy of the Anderson model

Using equation (9), we can determine the exact solutions of the Anderson Hamiltonian:

$$\Gamma^{(1)}_{dd,\sigma}(\omega) = \frac{\langle n_{d-\sigma}\rangle}{\omega - \varepsilon_d - U - \sum_k V_{kd}^2/(\omega - \varepsilon_k)} \tag{10}$$

$$G^{(1)}_{dd,\sigma}(\omega) = \frac{1 - \langle n_{d-\sigma}\rangle}{\omega - \varepsilon_d - \sum_k V_{kd}^2/(\omega - \varepsilon_k)} + \frac{\langle n_{d-\sigma}\rangle}{\omega - \varepsilon_d - U - \sum_k V_{kd}^2/(\omega - \varepsilon_k)} \tag{11}$$

$$G^{(2)}_{kd,\sigma}(\omega) = \frac{V_{kd}}{\omega - \varepsilon_k} G^{(1)}_{dd,\sigma}(\omega) \tag{12}$$

$$G^{(3)}_{kk,\sigma}(\omega) = \frac{1}{\omega - \varepsilon_k} + \frac{V_{kd}}{\omega - \varepsilon_k} G^{(2)}_{kd,\sigma}(\omega). \tag{13}$$

In order to calculate the ground-state energy, we take the density of the conduction band as

$$\rho(\varepsilon_k) = \begin{cases} \rho_0 & |\varepsilon_k| < D/2 \\ 0 & \text{otherwise} \end{cases} \tag{14}$$

and assume that $V_{kd}^2 = V^2$ and $D \gg |\varepsilon_d|$, U, V. Thus, according to the above equations, the ground-state energy of the Anderson model can be given as

$$\begin{aligned} E_{\mathrm{g}} \equiv \langle H\rangle(T=0) = {} & E_{\mathrm{g}}(U=0) + 2(\varepsilon_d - \varepsilon_f)\langle n_{d\sigma}\rangle + \frac{U}{\pi}\langle n_{d\sigma}\rangle \cot^{-1}\left(\frac{U + \varepsilon_d - \varepsilon_f}{\Delta}\right) \\ & + \frac{\Delta}{\pi}(1 - \langle n_{d\sigma}\rangle)\ln\left(1 + \frac{(\varepsilon_f - \varepsilon_d)^2}{\Delta^2}\right) + \frac{\Delta}{\pi}\langle n_{d\sigma}\rangle \ln\left(1 + \frac{(\varepsilon_f - \varepsilon_d - U)^2}{\Delta^2}\right) \end{aligned} \tag{15}$$

where $E_{\mathrm{g}}(U = 0)$ and Δ are taken from the work of Yamada [2]. In the calculation U is limited to a finite quantity.

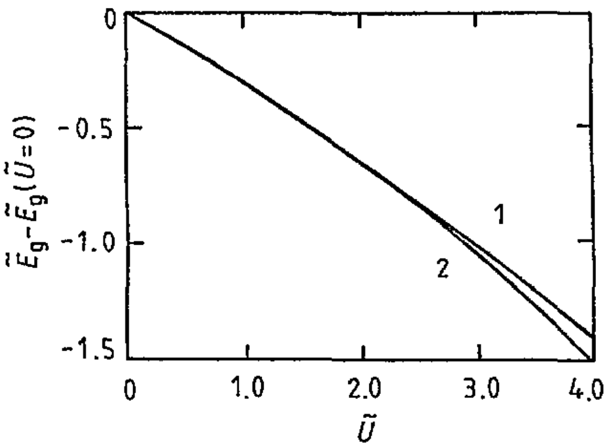

Figure 1. Plots of the ground-state energies given by Yamada (curve 1) and equation (16) (curve 2).

In the following we take the symmetric Anderson model [2] (i.e. $\varepsilon_d + U/2 = \varepsilon_f$) for example. If we introduce the reduced quantity $\tilde{C} = C/\pi\Delta$, the ground-state energy can be written as

$$\tilde{E}_{\mathrm{g}} = \tilde{E}_{\mathrm{g}}(\tilde{U}=0) - \frac{\tilde{U}}{4} - \frac{\tilde{U}}{2\pi}\tan^{-1}\left(\frac{\pi\tilde{U}}{2}\right) + \frac{1}{\pi^2}\ln\left(1+\frac{\pi^2\tilde{U}^2}{4}\right). \tag{16}$$

Here we compare the ground-state energies given by Yamada [2] and equation (16) for the symmetric Anderson model, which may be obtained from the work of Kawakami and Okiji [8] (figure 1). According to [8], we have found that the result of this paper does coincide with that of the Bethe *ansatz*.

4. Conclusions

This paper has some important results. First, the equation proved in this paper has provided an important way of solving some statistical models. Then, with the help of this equation, we have exactly solved the Anderson model and obtained the exact analytical expression of the ground-state energy. In particular, we have obtained this quantity in the symmetric Anderson model.

Acknowledgments

The author would like to thank Professor Xi-te Zheng, Professor Kai Chen, Professor Bin-jun Liu, Professor Zhong-cheng Wang, Professor Zheng-zhong Li, Dr Hong-xing Meng, Dr Hong-yu Ding and Dr Gou-ming Xiong for their encouragement and for valuable discussions.

References

[1] Anderson P W 1961 *Phys. Rev.* **124** 41
[2] Yamada K 1975 *Prog. Theor. Phys.* **53** 970
[3] Haldane F D M 1978 *Phys. Rev. Lett.* **40** 416
[4] Krishna-Murthy H R, Wilkins J W and Wilson K G 1975 *Phys. Rev. Lett.* **35** 1101
[5] Andrei N 1980 *Phys. Rev. Lett.* **45** 379
[6] Wiegmann P B 1980 *JETP Lett.* **31** 392
[7] Zubarev D N 1960 *Usp. Fiz. Nauk.* **71** 71
[8] Kawakami N and Okiji A 1981 *Phys. Lett.* **86A** 483