Electron localization and replica symmetry breaking in the quasicrystal-like system

I. Kanazawa [a,1]

[a] *Department of Physics, Tokyo Gakugei University, Koganei-shi, Tokyo 184-8501, Japan*

Abstract

We introduce the order parameter, which means replica symmetry breaking state in the transport property, in the quasicrystal-like system by using the effective Lagrangian of diffusion models.

Key words: quasicrystal; electron localization; replica symmetry breaking

1. Introduction

Recentry the present author [1,2] has considered the transport property in the randomly distributed system of the correlated configurations (the aggregation), in which the nearest distance between each configration is $\sim 2\pi/2k_{\rm F}$ (the quasicrystal-like state). It is known that the mean-free path of electrons in quasicrystals is short. Thus, the transport property in the quasicrystal-like system might be much referential to one in the quasicrystal system. In this study, we will introduce the order parameter, which means replica symmetry breaking state in the transport property, in the quasicrystal-like system by using the effective Lagrangian of diffusion models, taking into account the *sp*-*d* hybrization.

2. A Model System

In the quasicrystal-like state, we shall consider the effect of the $2k_{\rm F}$ phase shift scattering by the randomly distributed aggregation composed of correlated N number of configurations such as the prolate and oblate rhombohadra, in which the nearest distance between each configuration is $\sim 2\pi/2k_{\rm F}$ in the Feynman graph of Langer-Neal correction [3] with thermal Green function technique. If the d orbitals of the transition metal atoms located in unit-cell configurations are coupled with sp antibonding states, the partial density of sp states is increased below the Fermi energy which is in the pseudogap. The $2k_{\rm F}$ phase shift scattering enhances strongly the density wave of sp electrons with wave length $\sim 2\pi/2k_{\rm F}$. When a high density region of the standing wave is formed on the transition metal atom, the sp electrons hybrize more strongly the d orbitals of the transition metal atoms located in the configuration. Thus $2k_{\rm F}$ phase shift scattering and the *sp*-*d* hybrization are strongly correlated with each other. In this case, $\gamma \propto n_i N |V_{d,sp}|^2$ becomes large, where the matrix element $V_{d,sp}$ represents the *sp*-*d* hybrization, and n_i is the density of the aggregation, which is composed of N configurations connected with distance $\sim 2\pi/2k_{\rm F}$. The aggregation might be identified as the icosahedral cluster such as the Bergman type and the Mackay type [4,5]. N depends on the kind of materials.

To obtain the correct statistics we can obtain the Lagrangian of the diffusion mode by integrating over the classical Fermi fields [6]. To average over the randomly distributed aggregation, which is composed of N configurations connected with distance $\sim 2\pi/2k_{\rm F}$, we use the replica method [7]. We calculate the partition function Z_n of n replicas of the system and average Z_n over the aggregations such the icosahedral clusters. Performing averageing over the aggregation such as the icosahedral cluster, the potential will be regarded as a random

[1] E-mail:kanazawa@u-gakugei.ac.jp

quantity with a Gaussian δ-correlated distribution

$$\langle V(r)V(r')\rangle = \frac{n_i N|V_{d,sp}|^2}{2\pi\nu}\delta(r-r'), \tag{1}$$

when $V(r)$ is the effective potential of the clusters, and ν is the state density at T. Averaging Z_n over the distributions (3), we obtain

$$\langle\langle Z_n\rangle\rangle = \int \exp(S)\prod_a \mathrm{d}\bar{\psi}^a \mathrm{d}\psi^a,$$

$$S = \int \mathrm{d}r\left[\sum_{n,a}\left[\bar{\psi}_n^a(i\varepsilon_n + \frac{1}{2m}\Delta + \mu)\right]\psi_n^a + \frac{n_i N|V_{d,sp}|^2}{4\pi\nu}(\bar{\psi}\psi)^2\right], \tag{2}$$

where

$$\exp\left[\frac{n_i N|V_{d,sp}|^2}{4\pi\nu} \cdot\frac{1}{\Omega}\sum_{P_1,P_2,k}(\bar{\psi}_{P_1}\psi_{P_2})(\bar{\psi}_{P_2+k+2k_{\mathrm{F}}}\psi_{P_1-k-2k_{\mathrm{F}}})\right]$$
$$= \int \exp\left\{-\int\left[\frac{\pi\nu n_i N|V_{d,sp}|^2}{4}\mathrm{Sp}Q^2 - \frac{i}{2}n_i N|V_{d,sp}|^2(\bar{\psi}Q\psi)\right]\cdot\mathrm{d}r\right\}\prod \mathrm{d}Q$$
$$\cdot\left[\int \exp\left(-\int\frac{\pi\nu n_i N|V_{d,sp}|^2}{4}\mathrm{Sp}Q^2\mathrm{d}r\right)\prod \mathrm{d}Q\right]^{-1}. \tag{3}$$

Here,

$$\bar{\psi}Q\psi = \sum \psi_n^{a\dagger}Q_{nm}^{ab}\psi_m^b,\ \mathrm{Sp}Q^2 = \sum Q_{nm}^{ab}Q_{mn}^{ba}.$$

Where a and b are replica indies, and n and m are energy states. The longitudinal variations of Q make a large contribution to the free energy, so that these fluctuations can be neglected. As a result, the problem of electron diffusion reduces to a matrix non-linear sigma model

$$F \sim T\frac{\pi\nu}{4}\int\left[\mathrm{D}_{eff}\mathrm{Sp}(\nabla Q)^2 - 4\mathrm{Sp}(\varepsilon Q)\right]\mathrm{d}r, \tag{4}$$

where the effective diffusivity $\mathrm{D_{eff}} \sim \frac{v_{\mathrm{F}}^2}{3n_i N|V_{d,sp}|^2}$ and v_{F} is the Fermi velocity. This means that the *sp*-*d* hybridisation reduces strongly the diffusivity of electrons.

Using the analogy of the spin by Wegner [8], we can show the relation,

$$\begin{aligned}\bar{\psi}Q\psi &= \sum_{\substack{ab\\nm}}\psi_n^{a\dagger}Q_{nm}^{ab}\psi_m^b \\ &= \sum_{\substack{ab\\nm}}\psi_n^{a\dagger}\psi_n^a\sigma_a\psi_n^{a\dagger}\psi_m^b\sigma_b\psi_m^{\dagger b}\psi_m^b \\ &= \sum_{\substack{ab\\nm}}\left|\psi_n^a\right|^2 q_{nm}^{ab}\left|\psi_m^b\right|^2 = \sum_{\substack{ab\\nm}}P_n^a q_{nm}^{ab}P_m^b.\end{aligned} \tag{5}$$

Where σ_a (σ_b) is the set of Pauli matrices, $P_n^a = \left|\psi_n^a\right|^2$, $P_m^b = \left|\psi_m^b\right|^2$, and $q_{nm}^{ab} \equiv \sigma_a\psi_n^{a\dagger}\psi_m^b\sigma_b$. P_n^a means the probability that the state (the replica indice, a, and the energy level, n,) is one of different valleys. The overlap function, $P(q)$, and $\bar{q}$ are defined as follows,

$$P(q) = \left\langle\sum_{\substack{ab\\nm}}P_n^a P_m^b\delta\left(q - q_{nm}^{ab}\right)\right\rangle_{\mathrm{av}}$$

and

$$\bar{q} \equiv \left\langle\sum_{\substack{ab\\nm}}P_n^a q_{nm}^{ab}P_m^b\right\rangle_{\mathrm{av}},$$

where $\langle\ \rangle_{\mathrm{av}}$ is represents the bond averaged quantity. By using the overlap function $P(q)$, we can introduce the relation, $\bar{q} = \int_0^{q_{\max}}\mathrm{d}q\ q\ P(q)$.

Almost insulating quasicrystal-like system might mean the broadly distributed overlap function, $P(q)$, which corresponds to the replica symmetry breaking states.

3. Conclusion

We have introduced the order parameter, which means replica symmetry breaking state in the tranport property, in the quasicrystal-like system.

References

[1] I. Kanazawa, Physica B**284-288** (2000) 1161.

[2] I. Kanazawa, J. of Alloys and Compounds. in press.

[3] J. S. Langer and T. Neal, Phys. Rev Lett. **16** (1996) 984.

[4] C. Jarot, Phys. Rev. B**53** (1996) 181.

[5] A. Katz and D. Gratias, J. Non-Cryst. Solids **153-154** (1993) 187.

[6] K. B. Efetov, A. I. Laekin and D. E. Khmel'niskii, Zh, Eksp. Teor. Fiz. **79** (1980) 1120.

[7] S. F. Edwards, J. Phys. C**8** (1975) 1660.

[8] F. Wegner, Z. Physik B**35** (1979) 207.