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The adiabatic connection between the resonating-valence-bond state and the ground state of the half-filled periodic Anderson model

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Abstract. A one-parameter family of models interpolates between the periodic Anderson model with infinite repulsion at half-filling and a model whose ground state is exactly the resonating-valence-bond state. It is shown numerically that the excitation gap does not collapse. Therefore the ground states of the two models are adiabatically connected.

Recently correlation effects in electronic systems have been studied extensively. This is an old problem; however, it still is supplying interesting new physics, both experimentally and theoretically.

One can divide the ground states of strongly correlated systems into two groups. One is a metallic state which has a gapless excitation. The Fermi liquids and the Tomonaga–Luttinger liquids in one dimension are in this class. The other is an insulator which has a finite excitation gap. A simple example is a band insulator. There is another type of insulator which is caused by correlation (a Mott insulator). A well-known example of the correlated insulators is the half-filled Hubbard model in one dimension. Another example with a gap caused by the correlation is the half-filled Kondo lattice in one dimension. The charge degrees of freedom on the sites with on-site Coulomb repulsion are frozen. In this model both the charge and the spin degrees of freedom have a finite excitation gap though the lowest one is the spin excitation [1]. The periodic Anderson model which we investigate is a model in which the charge degree of freedom is also active.

The principle of adiabatic continuation is important in condensed matter physics. For example, the basic assumption of Fermi liquid theory is that the interacting system with quasiparticles is adiabatically connected to the non-interacting system with several phenomenological parameters. More specifically, the non-interacting fermions have a one-to-one correspondence with the quasiparticles. There is no level crossing in the process of increasing the interaction from zero to the full strength. Another notable example is the theory of the fractional quantum Hall effect. The adiabatic transformation in which the external magnetic fluxes are added to the electrons to become bosons [2] or composite fermions [3] is the crucial assumption.

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In this paper we choose the model of Strack [4] in one dimension as the canonical system with the correlation gap. The ground state is exactly the resonating-valence-bond (RVB) state [4–8]. See, e.g., reference [9] for the form of the RVB state. In this model, some of the correlation functions are obtained exactly [7, 8]. Moreover it is connected to the periodic Anderson model in one dimension as a parameter is varied. The periodic Anderson model has been commonly used to describe the correlation effects in heavy-fermion compounds and it reduces to the Kondo lattice model when the valence fluctuation is prohibited [1]. In order to clarify the relationship between the two models we numerically obtain the ground-state energy and the excitation gap for intermediate Hamiltonians.

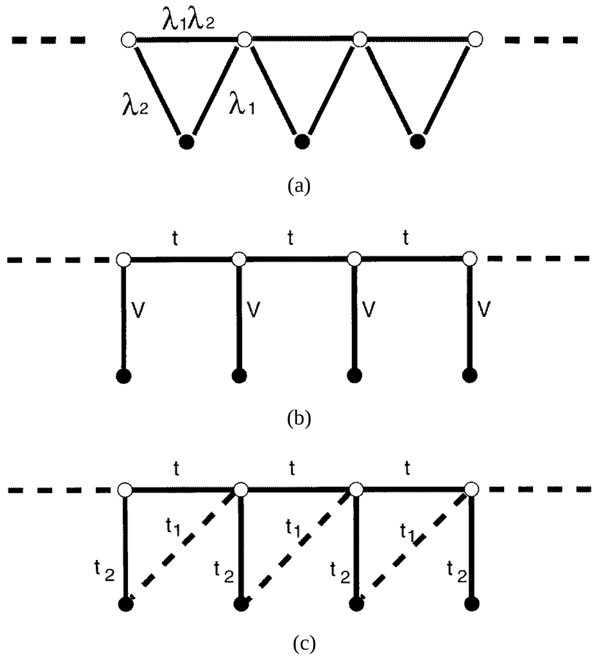

Figure 1. Lattice structure: (a) the Strack model, (b) the periodic Anderson model, and (c) an intermediate model connecting (a) and (b).

The Hamiltonian of the Strack model is

$$H_{ST} = \wp \sum_{n,\sigma} \{(-\lambda_1\lambda_2 c^\dagger_{n+1,\sigma} c_{n,\sigma} - \lambda_1 c^\dagger_{n+1,\sigma} f_{n,\sigma} - \lambda_2 c^\dagger_{n,\sigma} f_{n,\sigma} + \mathrm{HC}) + \epsilon^c c^\dagger_{n,\sigma} c_{n,\sigma} + \epsilon^f f^\dagger_{n,\sigma} f_{n,\sigma}\} \wp \quad (1)$$

where n is an index of the unit cell. In figure 1(a), the lattice structure of the model is shown where $\circ$ and $\bullet$ denote c- and f-sites respectively. Electrons at f-sites feel an infinitely large on-site Coulomb repulsion ($U = \infty$) and c-sites have no Coulomb repulsion ($U = 0$). The projection operator $\wp$ projects out the states with doubly occupancy at the f-sites. When one imposes $\epsilon^c = 2 - (\lambda_1^2 + \lambda_2^2)$, and $\epsilon^f = 2 - 2 = 0$, the ground state at half-filling is explicitly written as

$$|\Phi_G\rangle = \wp \prod_{n,\sigma} (\lambda_1 c^\dagger_{n,\sigma} + \lambda_2 c^\dagger_{n+1,\sigma} + f^\dagger_{n,\sigma})|0\rangle$$

$$= \prod_n (\lambda_1\lambda_2 d^\dagger_{c_n,c_{n+1}} + \lambda_1^2 d^\dagger_{c_n,c_n} + \lambda_2^2 d^\dagger_{c_{n+1},c_{n+1}} + \lambda_1 d^\dagger_{c_n,f_n} + \lambda_2 d^\dagger_{f_n,f_{n+1}})|0\rangle \quad (2)$$

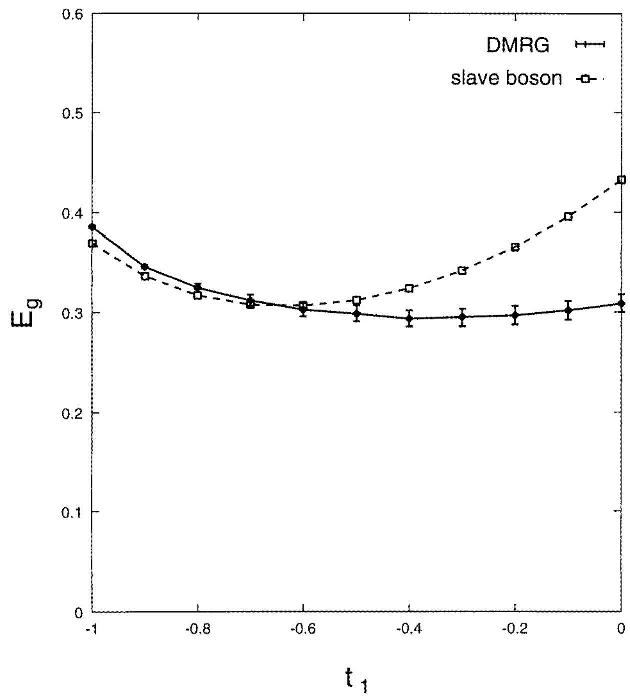

Figure 2. The excitation gap versus t_1.

where

$$d^{\dagger}_{\alpha_i,\beta_j} = \begin{cases} \alpha^{\dagger}_{i,\uparrow}\beta^{\dagger}_{j,\downarrow} + \alpha^{\dagger}_{j,\uparrow}\beta^{\dagger}_{i,\downarrow} & \text{for } i \neq j \\ \alpha^{\dagger}_{i,\uparrow}\alpha^{\dagger}_{i,\downarrow} & \text{for } i = j. \end{cases} \tag{3}$$

Note that the half-filling condition is that the number of electrons is one for each unit cell on average. This means that the conduction band is at half-filling as a single-band model if one fills each f-site with one electron. (Of course, the charge at the f-site can move and the spins at the f-site can flip using the double occupancy of the c-sites.) Thus the ground state is given by creations of nearest-neighbour singlet pairs in the vacuum. This state is the RVB state which we use as the canonical ground state with the correlation gap.

The existence of the finite energy gap has not been shown analytically, but it is numerically confirmed in the present work. This is consistent with the behaviour of correlation functions of local quantities which are analytically shown to be exponentially decaying [7, 8]. One can expect that the excitation above the ground state is closely related to a local singlet–triplet excitation which apparently has a finite energy cost.

The Hamiltonian of the periodic Anderson model is written as

$$\begin{aligned} H_{PA} = t\sum_{n,\sigma}(c^{\dagger}_{n+1,\sigma}c_{n,\sigma} + \mathrm{HC}) + V\sum_{n,\sigma}(c^{\dagger}_{n,\sigma}f_{n,\sigma} + \mathrm{HC}) \\ + \epsilon^{f}\sum_{n,\sigma}f^{\dagger}_{n,\sigma}f_{n,\sigma} + U\sum_{n}f^{\dagger}_{n,\uparrow}f_{n,\uparrow}f^{\dagger}_{n,\downarrow}f_{n,\downarrow} \end{aligned} \tag{4}$$

where U is the on-site Coulomb repulsion at f-sites. We consider the strong-coupling limit $U \to \infty$.

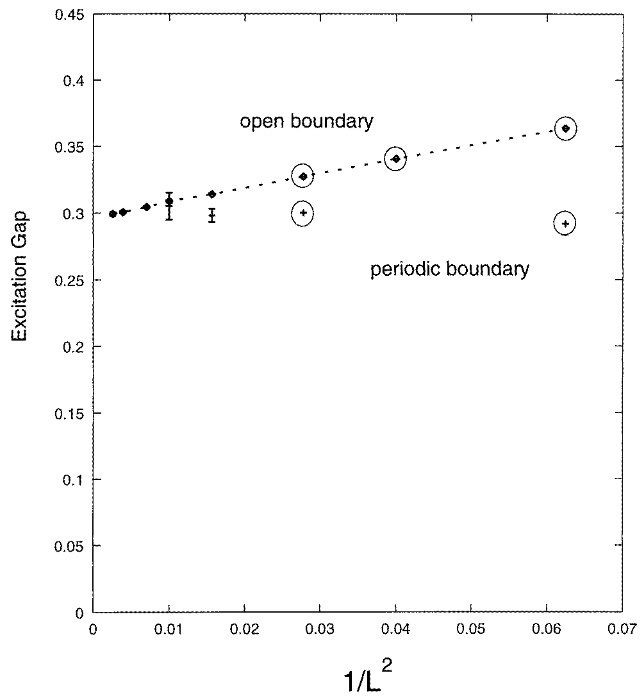

Figure 3. The excitation gap versus $1/L$; L is the system size.

These two Hamiltonians (1) and (4) are connected by changing hopping elements of the Strack model as shown in figure 1(c).

The intermediate Hamiltonian that we study is

$$H_C = \wp \sum_{n,\sigma} [(t c^\dagger_{n+1,\sigma} c_{n,\sigma} + t_1 c^\dagger_{n+1,\sigma} f_{n,\sigma} + t_2 c^\dagger_{n,\sigma} f_{n,\sigma} + \mathrm{HC}) + \epsilon^c c^\dagger_{n,\sigma} c_{n,\sigma} + \epsilon^f f^\dagger_{n,\sigma} f_{n,\sigma}]\wp. \quad (5)$$

The Strack Hamiltonian (1) is given by setting t_1 and t_2 as $t = -\lambda_1\lambda_2$, $t_1 = -\lambda_2$, $t_2 = -\lambda_1$. Also, when $t_1 = 0$, it reduces to the periodic Anderson model (4) with $U = \infty$.

To calculate the ground states and the energy gaps for sufficiently large systems, we used White's method (the DMRG) [10, 11]. Also numerical diagonalizations were performed for relatively small systems to check the validity of the DMRG results. It is interesting to note that DMRG is exact in the Strack model [13]. This fact supports the locality of the RVB state.

First we start with the Strack model by setting $t = t_1 = t_2 = -1$ and $\epsilon^c = \epsilon^f = 0$ in (5). Then it is identical to Strack's Hamiltonian (1) with $\lambda_1 = \lambda_2 = 1$. By changing t_1 while keeping the other parameters fixed in H_C, one gets the periodic Anderson model with $\epsilon^f = 0$ when $t_1 = 0$.

The excitation gaps obtained numerically are plotted in figure 2. They interpolate $t_1 = -1$ (the Strack model) and $t_1 = 0$ (the periodic Anderson model). We used a periodic boundary condition and each of the values is calculated by extrapolating to infinite system size. As a reference, the energy gap obtained by the slave-boson method is also plotted [13].

The system size dependence of the energy gap is shown in figure 3 with the results with open boundary conditions for the periodic Anderson model ($t_1 = 0$ in (5)).

As shown in figure 2, the excitation gap of the half-filled periodic Anderson model is connected to that of Strack's model without gap closing. This implies that the ground state of the periodic Anderson model at half-filling may have a close connection to that of the RVB state. For example, both ground states are singlets and have local nature. The excitations are expected to be closely related to local singlet–triplet excitations.

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