Perturbation study of the conductance through a finite Hubbard chain

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Abstract

The dc conductance through a Hubbard chain of size \(N(=1,2,3,\ldots)\) connected to noninteracting leads is studied at \(T=0\) in an electron-hole symmetric case using a perturbation theory in \(U\). The result shows a typical even-odd property corresponding to a Kondo or Mott-Hubbard physics.

Keywords: quantum transport; electron correlation; Fermi liquid; mesoscopic system

Motivated by a current interest in effects of electron correlation on the transport through small systems, we have examined some theoretical approaches [1,2]. In this report, using a perturbation approach, we study the size \((N)\) dependence of the transport through a small interacting chain connected to semi-infinite leads.

We start with the Hamiltonian \(\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_I\),

\[
\mathcal{H}_0 = -\sum_{i=-\infty}^{+\infty} t_i \left( c_{i+1\sigma}^\dagger c_{i\sigma} + c_{i\sigma}^\dagger c_{i+1\sigma} \right) -\mu \sum_{i=-\infty}^{+\infty} n_{i\sigma} + \sum_{j=1}^{N} \left( \epsilon_0 + \frac{U}{2} \right) n_{j\sigma},
\]

\[
\mathcal{H}_I = U \sum_{j=1}^{N} \left[ n_{j\uparrow} n_{j\downarrow} - \frac{1}{2} (n_{j\uparrow} + n_{j\downarrow}) \right].
\]

Here \(c_{i\sigma}^\dagger\) is a creation operator for an electron with spin \(\sigma\) at site \(i\), \(n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}\). The hopping matrix element is uniform \(t_i = t\) except at the boundaries between the central region and two leads; \(t_0 = v_L\) and \(t_N = v_R\).

At \(T=0\), the dc conductance \(g_N\) can be written in term of an inter-boundary element of a single-particle Green’s function \(G_{N1}(\omega + i0^+)\), and is determined by the value at the Fermi level \(\omega = 0\) as \(g_N = (2e^2/h) 4 \Gamma_L(0) \Gamma_R(0) |G_{N1}(i0^+)|^2\) [1]. Here \(\Gamma_{\alpha}(0) = \pi D(0) v_\alpha^2\) with \(\alpha = L, R\), and \(D(0) = \sqrt{4t^2 - \mu^2} / (2\pi t^2)\). The assumption made here is the validity of the perturbation theory in \(U\). This seems to be probable for small \(N\). In that case, the self-energy due to \(\mathcal{H}_I\) has a property \(\text{Im} \Sigma_{j\uparrow}(i0^+) = 0\) at \(T = 0\) [3], and \(g_N\) can be obtained through a scattering problem of free quasi-particles [2].

In this report, we consider an electron-hole symmetric case taking the parameters to be \(\mu = 0\) and \(\epsilon_0 + U/2 = 0\). If the system has an additional in-
version symmetry $v_L = v_R$, it can be shown that a perfect transmission occurs $g_N \equiv 2e^2/h$ for odd $N (= 2M + 1)$ independent of the values of $U$ and $M$ [2]. This is caused by the Kondo resonance appearing at the Fermi level for odd $N$.

On the other hand, for even $N$, we evaluate the self-energy $\Sigma_{ij}(\omega^\pm)$ within the second order in $U$ at $\omega = 0$, and then obtain $G_{N1}(\omega^\pm)$ solving the Dyson equation in the real space [2]. In Fig. 1, $g_N$ for even $N (= 2M)$ is plotted vs $M$ for several values of $v_L (= v_R)$, where $U/(2\pi t) = 1.0$. The dc conductance decreases with increasing the size $2M$. This behavior can be regarded as a tendency toward a Mott-Hubbard insulator, and it is pronounced for larger $U$. In Fig. 2, $g_N$ for even $N (= 2, 4, \ldots)\) is plotted vs $U$. The value of $g_{2M}$ decreases with increasing $U$. When $v_L$ (or $v_R$) is smaller than $t$, the reduction of $g_{2M}$ is proportional to $U^2$ at $U/(2\pi t) \ll 1$. As it is seen in the plots for $v_L = v_R = 0.7t$ (dashed lines), the peak structure in the $U$ dependence becomes sharp for large $M$, and in the limit $M \to \infty$ the peak seems to vanish leaving the value at a singular point $U = 0$ unchanged. In contrast, in the case of $v_L = v_R = t$ (solid lines), the reduction of $g_{2M}$ is proportional to $U^4$ at $U/(2\pi t) \ll 1$, and $g_{2M}$ seems to be finite in the limit of large $M$. However, in order to verify this behavior for large $M$, the contributions of the higher-order terms should be examined because the unperturbed Hamiltonian $\mathcal{H}_0$ has a translational invariance accidentally in this case.

Qualitatively, the even-odd property seems to be understood from that in the unperturbed system, especially from the level structure of the isolated chain. For odd $N$, there is a semi-occupied one-particle state at the Fermi level $\omega = 0$, and thus a doublet ground state is realized. When the leads are connected, the ground state is replaced by a Kondo singlet state and contributes to the tunneling. On the other hand, for even $N$, the Fermi level lies between the highest occupied level and the lowest unoccupied level, and thus a finite energy corresponding to the gap is necessary to excite the electrons. Although the levels are broadened by the coupling with the leads, the even-odd property is determined by whether there exists a zero-energy excitation or not. At finite temperatures, a characteristic energy scale of the Kondo or Mott-Hubbard physics will play an important role.

We expect that the model and approach used here can be applied to a series of quantum dots or a quantum wire of nanometer scale.

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References

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