Complementary inequality between the energy gap and fluctuation

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We present an upper bound on the energy gap above the ground energy in terms of the fluctuation of the particle position in one-particle tight-binding systems. We here consider the ground state of general one-dimensional tight-binding systems, whose the Hamiltonian is given by

\[ H = \sum_{x=1}^{L} (u_x a_x^\dagger a_x + v_x a_{x+1}^\dagger a_x + v_x^* a_x^\dagger a_{x+1}) \]  (1)

with \( a_{L+1} = a_1 \). We can extend the following result to higher-dimensional systems.

We then define an operator \( F \) as

\[ F \equiv \sum_{x=1}^{L} f(x) |x\rangle \langle x|, \]

where \( f(x) \) is a periodic real function:

\[ f(x+L) = f(x). \]

For example, if we choose \( f(x) = x \), we can regard \( X \equiv \sum_{x=1}^{L} x |x\rangle \langle x| \) as the position operator. Then, the energy gap \( \delta E_0 \) satisfies the inequality

\[ \delta E_0 \leq \frac{|\langle \psi_0 | H_{OD} | \psi_0 \rangle|}{2(\Delta F)^2}, \]  (2)

where \( |\psi_0\rangle \) is the ground state and \( H_{OD} \equiv \sum_{x=1}^{L} f(x+1) - f(x)^2 (v_x a_x^\dagger a_{x+1} + \text{c.c.}) \).

Our inequality gives a complementary relationship between the energy gap and the localization of the particle; that is, the energy gap narrows as the ground state spreads spatially, while the energy gap can broaden as the ground state becomes localized. We compare our upper bound with the energy gap which we calculated numerically exactly in one and two dimensions; this comparison confirms that our upper bound indeed places a tight restriction on the energy gap.

We also extend the inequality (2) to many-body systems with Hamiltonians which contain terms of up to \( \kappa \)-body coupling with finite \( \kappa \):

\[ H = \sum_{i_1 < i_2 < \cdots < i_N} \sum_{\mu_1, \ldots, \mu_N} J_{i_1, \ldots, i_N}^{\mu_1, \ldots, \mu_N} s_{i_1}^{\mu_1} \otimes \cdots \otimes s_{i_N}^{\mu_N}, \]  (3)

where \( \{ s_{i}^{\mu} \}_{\mu,i} \) are operator bases at the site \( i \); for spin \((1/2)\) systems, for example, \( \{ s_{i}^{\mu} \}_{\mu,i} = \{ \sigma_{i}^{x}, \sigma_{i}^{y}, \sigma_{i}^{z} \} \) with \( \{ \sigma_{i}^{\mu} \}_{\mu=x,y,z} \) the Pauli matrices. We then make the fluctuation \( \Delta X \) of the particle position correspond to the fluctuation \( \Delta A \) of an extensive quantity \( A \), which is defined as \( A = \sum_{i=1}^{N} a_i \) with \( a_i = \sum_{\mu} a_i^{\mu} s_{i}^{\mu} \) and \( \| a_i \|_2 = 1 \). In the case of a spin \((1/2)\) system with \( a_i = \sigma_{i}^{z} \), the operator \( A \) reduces to the magnetization along the \( z \)-axis, namely \( A = \sum_{i=1}^{N} \sigma_{i}^{z} \). Then, the corresponding inequality to (2) is given by

\[ \delta E_0 \leq c_0 \frac{\| H \|_2}{(\Delta A)^2}, \]  (4)

with \( c_0 \) a constant and \( \| H \|_2 \) the spectral norm of the Hamiltonian.