On the relation between entanglement and subsystem Hamiltonians

INGO PESCHEL1(a) and MING-CHIANG CHUNG2,3

1 Fachbereich Physik, Freie Universität Berlin - Arnimallee 14, D-14195 Berlin, Germany
2 Physics Division, National Center for Theoretical Science - Hsinchu 30013, Taiwan
3 Institute of Physics, Academia Sinica - Taipei 11529, Taiwan

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Abstract – We show that a proportionality between the entanglement Hamiltonian and the Hamiltonian of a subsystem exists near the limit of maximal entanglement under certain conditions. Away from that limit, solvable models show that the coupling range differs in both quantities and allow to investigate the effect.

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Introduction. – The reduced density matrix (RDM) which describes a subsystem \( \alpha \) of a total system in a pure quantum state has been the topic of numerous studies. It can be written in the form \( \rho_\alpha = \exp(-\mathcal{H}_\alpha)/Z \) with an operator \( \mathcal{H}_\alpha \) which has become known as entanglement Hamiltonian [1]. For free fermionic or bosonic systems in their ground state, \( \mathcal{H}_\alpha \) has again free-particle form and can be determined explicitly, see [2] for a review. Because of the thermal form of \( \rho_\alpha \), the question whether \( \mathcal{H}_\alpha \) is related to the subsystem Hamiltonian \( \mathcal{H}_\alpha \) arises naturally. A certain type of relation has already been pointed out some time ago [3]. For hopping models, the correlation matrix which determines \( \mathcal{H}_\alpha \) can be viewed as a Hamiltonian where only two bands, corresponding to occupied and empty states, appear. Thus for insulators with two bands, it is a flat-band version of the physical Hamiltonian. This has been used to investigate the problem of zero modes in topological insulators, see, e.g., [4]. The considerations can be generalized also to cases with pair creation, see [5].

In this paper, however, we are interested in a more direct relationship like a proportionality between the two Hamiltonians. From the exact results, one sees that in general this does not exist. For example, segments in non-critical quantum chains like the transverse Ising model or a dimerized hopping model lead to a single-particle spectrum in \( \mathcal{H}_\alpha \) which is linear near zero, whereas \( \mathcal{H}_\alpha \) has energy bands with a gap. Moreover, the low-lying eigenfunctions of \( \mathcal{H}_\alpha \) are concentrated near the boundaries while they are extended in \( \mathcal{H}_\alpha \) except for zero-energy modes. A certain similarity exists only in the critical case, where both spectra are asymptotically linear with level spacing \( 1/\ln L \) and \( 1/L \), respectively, where \( L \) is the length of the subsystem. This allows to define an effective temperature in the RDM [6]. However, the eigenfunctions of the two Hamiltonians still differ, and also the forms of \( \mathcal{H}_\alpha \) and \( \mathcal{H}_\alpha \) in real space, see [2].

The situation becomes different if the subsystem is translationally invariant, as is the case for sublattices in a chain or for a leg of a ladder. Then the eigenfunctions of \( \mathcal{H}_\alpha \) and \( \mathcal{H}_\alpha \) are both momentum eigenstates and a closer relation is possible, although not necessary. For a transverse Ising chain, for example, the sublattices simply decompose into the individual sites, but \( \mathcal{H}_\alpha \) has non-trivial momentum-dependent excitations in the fermionic representation [7]. In other cases, however, correspondences between the spectra were found, see, e.g., [8,9] for quantum Hall systems and [10] for a Heisenberg ladder. This feature was explained in a recent paper for coupled conformally invariant subsystems with left- and right-moving particles [11].

In the present note, we want to point out that a relation \( \mathcal{H}_\alpha \sim \mathcal{H}_\alpha \) can be obtained very simply via perturbation theory for a total system formed from two strongly coupled subsystems. This is essentially also the case treated in [11]. We also show, for a solvable fermionic system, how away from strong subsystem coupling the operator \( \mathcal{H}_\alpha \) contains
longer-range interactions, as found numerically in [12] for Heisenberg and AKLT ladders.

**General result.** – Consider a quantum system made up of two parts with Hamiltonians $H_1$ and $H_2$ coupled via the Hamiltonian $H'$. This could be a ladder with two legs and rungs described by $H'$. We assume $H'$ large and treat $H_1 + H_2$ as a perturbation. Then, if $|\Psi_0\rangle$ is the (non-degenerate) ground state of $H'$, it changes in first order to

$$|\Psi_1\rangle = |\Psi_0\rangle - \sum_{k \neq 0} |\Psi_k\rangle \frac{\langle \Psi_k | (H_1 + H_2) | \Psi_0 \rangle}{E_k - E_0}, \quad (1)$$

where $|\Psi_k\rangle$ are the eigenfunctions of $H'$ and $E_k$ the eigenvalues. We now assume

1) there is only coupling to excited states with the same gap $\Delta = E_k - E_0$;

2) both $H_\alpha$ give the same matrix elements, i.e. $\langle \Psi_k | H_1 | \Psi_0 \rangle = \langle \Psi_k | H_2 | \Psi_0 \rangle$.

Then

$$|\Psi_1\rangle = |\Psi_0\rangle - \frac{2}{\Delta} \sum_{k \neq 0} |\Psi_k\rangle \langle \Psi_k | H_1 | \Psi_0 \rangle, \quad (2)$$

which can be written

$$|\Psi_0\rangle = |\Psi_0\rangle - \frac{2}{\Delta} \hat{H}_1 |\Psi_0\rangle, \quad (3)$$

where $\hat{H}_1 = H_1 - \langle H_1 \rangle$ with $\langle H_1 \rangle = \langle \Psi_0 | H_1 | \Psi_0 \rangle$. The total density matrix then is, to first order,

$$\rho^1 = \rho_1 - \frac{2}{\Delta} (\hat{H}_1 \rho_1 + \rho_1 \hat{H}_1), \quad (4)$$

Since $H_1$ operates only in subsystem 1, the trace over subsystem 2 can be taken and leads to

$$\rho_1^1 = \rho_1 - \frac{2}{\Delta} (\hat{H}_1 \rho_1 + \rho_1 \hat{H}_1), \quad (5)$$

where $\rho_1$ is the RDM for $|\Psi_0\rangle$. If now also the following holds:

3) $\rho_1$ is a multiple of the unit matrix,

one can pull $\rho_1$ out in front and write, exponentiating the differences,

$$\rho_1^1 = \rho_1 - \frac{2}{\Delta} (\hat{H}_1 \rho_1 + \rho_1 \hat{H}_1), \quad (5)$$

where $Z = \text{tr}_1 (1 - 4H_1/\Delta) = \text{tr}_1 \exp(-4H_1/\Delta)$. Thus $\rho_1^1$ is correctly normalized to first order and one has the relation

$$\hat{H}_1 = \frac{4}{\Delta} H_1 \quad (7)$$

*Heisenberg ladders.* – The conditions used in the above derivation may seem relatively restrictive. However, they are fulfilled for an antiferromagnetic Heisenberg ladder with Hamiltonian

$$H = H_1 + H_2 + H'$$

$$= J \sum_n S_n S_{n+1} + J' \sum_n T_n T_{n+1} + J'' \sum_n S_n T_n, \quad (8)$$

where the $S$ and $T$ are spin-one-half operators. Then the ground state $|\Psi_0\rangle$ is a product of singlets at the different rungs. Each singlet is maximally entangled and gives a RDM which is 1/2 times the 2 × 2 unit matrix. Each term in $H_\alpha$ has matrix elements to triplet states at two neighbouring rungs which leads to $\Delta = 2J'$. Thus the coupling in $H_1$ is given by $K = 4J/2J' = 2J'/J'$. This is exactly the result found numerically in [12] in the limit $J \ll J'$, see fig. 5(a) there. In their notation, $K = 2\cos\theta/\sin\theta$ and one has to consider $\theta \approx \pi/2$ where $K = (2/\pi - \theta)$. One can ask if the considerations also hold for an anisotropic Heisenberg model. If the rung coupling remains isotropic, this is indeed the case, since the singlet-triplet level scheme for each rung does not change. However, if $H'$ is of XXZ form, one has two single levels and one doublet. Then there are excitations with two different gaps to the spin singlet, which is the lowest state throughout the planar region $(|J'_x|, |J'_y|) \leq J'_x, J'_y$. These appear with different pieces of $H_1$ and (7) is changed to

$$\hat{H}_1 = \frac{4}{\Delta_{xy}} H_{1,xy} + \frac{4}{\Delta_z} H_{1,z}, \quad (9)$$

where $\Delta_{xy} = J'_x + J'_y$ and $\Delta_z = 2J'$. Thus while the Heisenberg form remains, the anisotropy of $H_1$ is not the same as that of $H_1$. An exception is the planar case, $H_{1,z} = 0$. Then $H_1$ couples only to the doublet and the formula (7) with the proper gap holds again. This is interesting, because $H_1$ is then solvable in terms of fermions whereas the Hamiltonian of the ladder is not.

*Fermionic systems.* – The considerations also apply to a fermionic system as treated in [11]. Consider two species of fermions with opposite dispersion and mutual coupling. The Hamiltonian $\hat{H} = H_1 + H_2 + H'$ is

$$H = \sum_q \gamma_q a_q^\dagger a_q - \sum_q \gamma_q b_q^\dagger b_q + \sum_q \delta (a_q^\dagger b_q + b_q^\dagger a_q), \quad (10)$$

where $q$ denotes the momentum. If $\gamma_q = q$, this describes two systems with only right- or left-moving particles. If $\gamma_q = \text{cos} q$, it describes a ladder with opposite nearest-neighbour hopping matrix elements in the two legs. The coupling term $H'$ is diagonalized by the operators $(a_q^\dagger \pm b_q)/\sqrt{2}$ and gives the two single-particle levels $\pm \delta$ for each $q$, thus $\Delta = 2\delta$. Moreover, the levels are analogous to spin singlets and therefore maximally entangled. The operators $H_\alpha$ have equal matrix elements between them. Therefore
On entanglement and subsystem Hamiltonians

Fig. 1: (Colour on-line) Dispersion relation for the single-particle excitations in $\mathcal{H}_1$ for the model (10) with $\gamma_q = -\cos q$ and several values of $\delta$. The dotted line shows a cosine for comparison.

(7) holds for large $\delta$ and $\mathcal{H}_1$ is of the form

$$\mathcal{H}_1 = \sum_q \varepsilon_q a_q^\dagger a_q$$

with $\varepsilon_q = 4\gamma_q/\Delta = 2\gamma_q/\delta$. This is the result found in [11].

For this system, however, $\mathcal{H}_1$ can be determined exactly and the $\varepsilon$ follow from the eigenvalues of the correlation matrix in the subsystem [2,13–15]. But because of the translation invariance, this matrix is diagonal in momentum space and the eigenvalues are given by the occupation numbers $n_q = \langle a_q^\dagger a_q \rangle$. Diagonalizing (10) with a canonical transformation $a_q = u_q \alpha_q + v_q \beta_q, b_q = -v_q \alpha_q + u_q \beta_q$ where $u_q^2 + v_q^2 = 1$, one obtains

$$H = \sum_q \omega_q (\alpha_q^\dagger \alpha_q - \beta_q^\dagger \beta_q), \quad \omega_q = \sqrt{\gamma_q^2 + \delta^2}.$$ (12)

This gives the occupation numbers

$$n_q = v_q^2 = \frac{1}{2} \left(1 - \frac{\gamma_q}{\omega_q}\right)$$

and leads to $\varepsilon_q = \ln[(1 - n_q)/n_q]$, or

$$\varepsilon_q = \ln \left(\frac{\omega_q + \gamma_q}{\omega_q - \gamma_q}\right).$$ (14)

In [11] this was obtained in a different way. If one considers the other subsystem, $u_q^2$ is replaced by $u_q^2$, which changes the sign of $\varepsilon_q$ but not the RDM spectrum.

Expanding (14) for large $\delta$, one reobtains the result $\varepsilon_q = 2\gamma_q/\delta$ found above. In the opposite case, $\delta \ll \gamma_q$, however, the variation is logarithmic, $\varepsilon_q = 2\ln(2\gamma_q/\delta)$. The variation of $\varepsilon_q$ with $q$ for $\gamma_q = -\cos q$ is shown in fig. 1 for several values of $\delta$. One sees that the amplitude increases as $\delta$ becomes smaller. At the same time, the curves deviate from a simple cosine function and become more rectangular. This is illustrated for $\delta = 0.1$ by the dotted line. Near the points $q = \pm \pi/2$, one is always in the strong-coupling limit and the slope is $\pm 2/\delta$.

The deviation of $\varepsilon_q$ from $\gamma_q$ means that the hopping in $\mathcal{H}_1$ is different from that in $\mathcal{H}_1$. In the example, where one has nearest-neighbour hopping in $\mathcal{H}_1$, one finds hopping to more distant sites in $\mathcal{H}_1$. This can be seen directly by expanding (14) to higher orders. It is more instructive, though, to perform a numerical Fourier transformation of $\varepsilon_q$ and to present the result graphically. This is done in fig. 2, where the amplitudes $t_n$ for hopping to the $n$-th neighbour are plotted, normalized by $t_1$. Shown are only those for odd distances, since the other ones are zero.

For large $\delta$, one sees a very rapid decrease of the $t_n$ with $n$ and only $t_1$ is relevant. As $\delta$ decreases, the decay slows down and also longer-range hopping becomes important. Due to the shape of $\varepsilon_q$, however, the dominant term is always $t_1$. Very similar results were obtained numerically in [12] for Heisenberg ladders. Formally, they are connected with the higher orders in the perturbation expansion for $|\Psi_0\rangle$. The effect is reminiscent of the situation for transfer matrices in two-dimensional Ising or Gaussian models, where the exact operators in the exponent and those of the Hamiltonian limit differ in dispersion relation and coupling range.

Concluding remarks. – Summing up, we have shown how a proportionality between $\mathcal{H}_1$ and $\mathcal{H}_1$ can be obtained for strongly coupled and maximally entangled subsystems by treating the subsystem Hamiltonians in first-order perturbation theory. Whether they describe a critical or a non-critical system does not matter, only their smallness enters. The entanglement is decreased only weakly in this case. The fermionic example showed explicitly how the situation changes away from the strong-coupling limit. In the free-fermion and free-boson case, one can find a number of simple systems, where an expression as (14) appears. Examples are hopping ladders with alternating rung couplings or the BCS model and the (bosonic) Luttinger model as systems of right- and left-moving...
particles. An exception is a homogeneous hopping ladder. There $H_1 + H_2$ commutes with $H'$ and does not change the wave function. The matrix elements in condition (2) are then of opposite sign.

Finally, one should mention that formulae similar to (13), (14) have appeared before in studies of quenches in quantum chains [16,17]. In this case, one determines the occupation numbers for the modes of the new Hamiltonian in the state before the quench, using the appropriate canonical transformation. If, for example, one starts in the ground state of a hopping chain with alternating site energies $\pm \delta$ and switches this dimerization off, as done in [16], the $n_q$ of the modes in the homogeneous chain are exactly (13) with $\gamma_q = \cos q$. As above, one can then define a thermal density matrix and an effective Hamiltonian, and the difference is only that these quantities refer to the full system and not to a part of it. The relation $\varepsilon_q = 2\gamma_q/\delta$ in this case was already noted in [2].

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