Entangled Quantum States and the Hubbard Model

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We describe criteria for separability for states in the Hilbert space $\mathbf{C}^m \otimes \mathbf{C}^n$ which is convenient for application in computer algebra. We use the requirements for a state in the Hilbert space $\mathbf{C}^m \otimes \mathbf{C}^n$ for $m, n \in \mathbf{N}$ to be entangled to find when states evolving under the Hubbard model become entangled. We apply this criteria to determine when states evolving under the Hubbard model become entangled. We also give a SymbolicC++ implementation of the criteria and its application to the Hubbard model. We identify subspaces for which separable states remain separable and subspaces for which entangled states remain entangled.

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two finite dimensional Hilbert spaces. The measure for entanglement for pure states $E(|u\rangle\langle u|)$ is defined as follows

$$E(|u\rangle\langle u|) := S_{\dim(\mathcal{H}_1)}(\rho_{\mathcal{H}_1}) = S_{\dim(\mathcal{H}_2)}(\rho_{\mathcal{H}_2})$$

where the density operators are defined as

$$\rho_{\mathcal{H}_1} := \mathrm{Tr}_{\mathcal{H}_2}|u\rangle\langle u|, \qquad \rho_{\mathcal{H}_2} := \mathrm{Tr}_{\mathcal{H}_1}|u\rangle\langle u|$$

and

$$S_b(\rho) := -\mathrm{Tr}\rho \log_b \rho.$$

We found an equivalent form for the criteria for entanglement which is easier to implement for computer algebra applications. Let $m := \dim(\mathcal{H}_1)$, $n := \dim(\mathcal{H}_2)$,

$$\{\, |j\rangle_{\mathcal{H}_1}\,, j = 0, 1, \ldots, m-1\,\}$$

be an orthonormal basis for $\mathcal{H}_1$ and

$$\{\, |j\rangle_{\mathcal{H}_2}\,, j = 0, 1, \ldots, n-1\}$$

be an orthonormal basis for $\mathcal{H}_2$. Thus

$$\{\, |j\rangle_{\mathcal{H}_1} \otimes |k\rangle_{\mathcal{H}_2}\,, j = 0, 1, \ldots, m-1\,, k = 0, 1, \ldots, n-1\}$$

is an orthonormal basis for $\mathcal{H}_1 \otimes \mathcal{H}_2$. We consider arbitrary normalized states $|z\rangle$ in the Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$ respectively. We can identify these states with the vectors $(z_0, z_1, \ldots, z_{nm-1})^T \in \mathbf{C}^{mn}$ as follows

$$|z\rangle := \sum_{i=0}^{m-1} \sum_{j=0}^{n-1} z_{in+j} |i\rangle_{\mathcal{H}_1} \otimes |j\rangle_{\mathcal{H}_2}, \qquad \sum_{j=0}^{nm-1} |z_j|^2 = 1.$$

Thus we see that the tensor product is equivalent to considering the Kronecker product. To ensure that $|z\rangle$ is a product state we must have

$$z_{in+j} z_{kn+l} = z_{in+l} z_{kn+j}$$

$$i = 0, 1, \ldots, m-1, \quad j = 0, 1, \ldots, n-1,$$

$$k = i+1, i+2, \ldots, m-1, \quad l = j+1, j+2, \ldots, n-1.$$

As an example we consider the Hubbard model. We wish to know when an entangled state results for given parameters t and U as well as the time τ required for the system to evolve to these states. SymbolicC++ can be used to implement our criteria. We describe a SymbolicC++ program which gives the equations for separability for given initial states under evolution of the Hubbard model.

Suppose $\hat{H}$ can be written as $A_1 \otimes I_2 + I_2 \otimes A_2$ where $A_1, A_2 \in M^2$ and I_2 is the 2 times 2 identity matrix. Then

$$\begin{aligned} \exp(-i\hat{H}\tau/\hbar) &= \exp(-i\hat{H}\tau/\hbar A_1 \otimes I_2 - i\hat{H}\tau/\hbar I_2 \otimes A_2) \\ &= \exp(-i\hat{H}\tau/\hbar A_1) \otimes \exp(-i\hat{H}\tau/\hbar A_2). \end{aligned}$$

In this case separable states remain separable under time evolution in the model, and entangled states remain entangled under time evolution in the model. For the two point Hubbard model we have

$$\hat{H} = tU_{NOT} \otimes I_2 + tI_2 \otimes U_{NOT} + \mathrm{diag}(U, 0, 0, U), \qquad U_{NOT} := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

The matrix $\mathrm{diag}(U, 0, 0, U)$ cannot be written in the form $A \otimes I_2 + I_2 \otimes B$. Thus we conclude that some initial separable states evolve into entangled states under time evolution in the model.