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Entanglement, Hubbard Model, and Symmetries

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Entangled quantum states are an important component of quantum computing techniques such as quantum error-correction, dense coding, and quantum teleportation. We use the requirements for a state in the Hilbert space $\mathbf{C}^2 \otimes \mathbf{C}^2$ to be entangled to find when states evolving under the two-point Hubbard model become entangled. We also investigate the connection of entanglement and discrete symmetries of the two-point Hubbard model. Furthermore we discuss the inclusion of phonon coupling.

KEY WORDS: entanglement; Hubbard model; phonon coupling.

Entanglement (Hardy and Steeb, 2001; Nielsen and Chuang, 2000; Preskill, 2001; Steeb and Hardy, 2000, 2002, 2004) is the characteristic trait of quantum mechanics which enforces its entire departure from classical lines of thought. We consider entanglement of pure states. Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two finite dimensional Hilbert spaces. Thus a basic question in quantum computing is as follows: given a normalized state $|u\rangle$ in the Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$, can two normalized states $|x\rangle$ and $|y\rangle$ in the Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ respectively be found such that

$$|x\rangle \otimes |y\rangle = |u\rangle. \tag{1}$$

In other words, what is the condition on $|u\rangle$ such that $|x\rangle$ and $|y\rangle$ exist? If no such $|x\rangle$ and $|y\rangle$ exist then $|u\rangle$ is said to be *entangled*. The measure for entanglement for pure states $E(|u\rangle\langle u|)$ is defined as follows (Hardy and Steeb, 2001; Nielsen and Chuang, 2000; Preskill, 2001; Steeb and Hardy, 2004)

$$E(|u\rangle\langle u|) := S_d(\rho_{\mathcal{H}_1}) = S_d(\rho_{\mathcal{H}_2}) \tag{2}$$

where $d = \min\{\dim(\mathcal{H}_1), \dim(\mathcal{H}_2)\}$ and the density operators are defined as

$$\rho_{\mathcal{H}_1} := \mathrm{tr}_{\mathcal{H}_2}|u\rangle\langle u|, \qquad \rho_{\mathcal{H}_2} := \mathrm{tr}_{\mathcal{H}_1}|u\rangle\langle u| \tag{3}$$

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and

$$S(\rho) := -\mathrm{tr}\rho \log_d \rho \tag{4}$$

and S denotes the von Neumann entropy. Here tr denotes the trace and $\mathrm{tr}_{\mathcal{H}_1}$ denotes the partial trace over $\mathcal{H}_1$.

The partial trace can also be calculated as follows. Let

$$|\psi\rangle = \sum_{j=0}^{n-1}\sum_{k=0}^{n-1} c_{jk}|j\rangle \otimes |k\rangle, \qquad \sum_{j=0}^{n-1}\sum_{k=0}^{n-1} c_{jk}c_{jk}^* = 1$$

be a pure state in the Hilbert space $\mathbf{C}^n \otimes \mathbf{C}^n$. We define the $n \times n$ matrix R as $R := (c_{jk})$, where $j, k = 0, 1, \ldots, n-1$. Then

$$\rho_{\mathcal{H}_1} = \mathrm{tr}_{\mathcal{H}_2}\rho = RR^\dagger.$$

Under a local unitary transformation $U_1 \otimes U_2$, the matrix R is changed to $R \to U_1^{\mathrm{T}} R U_2$. The reduced density matrix is thus transformed as

$$\rho_{\mathcal{H}_1} \to \left(U_1^{\mathrm{T}} R U_2\right)\left(U_2^\dagger R^\dagger U_1^{\mathrm{T}\dagger}\right) = U_1^{\mathrm{T}} R R^\dagger U_1^{\mathrm{T}\dagger}$$

since $U_1 U_2^\dagger = I_n$. The entanglement of an arbitrary density matrix defined above is related to a quantity called concurrence $C(\rho)$ (Wooters, 1998) by the function

$$S(\rho_{\mathcal{H}_1}) = h\left(\frac{1 + \sqrt{1 - C^2(\rho)}}{2}\right)$$

where $h(x) := -x\log_2 x - (1-x)\log_2(1-x)$. For a pure state with $n = 2$ the concurrence takes the form

$$C(|\psi\rangle\langle\psi|) = |\langle\psi|(\sigma_y \otimes \sigma_y)|\psi^*\rangle| = 2|c_{00}c_{11} - c_{01}c_{10}|.$$

We can use the concurrence directly as the measure of entanglement. If the concurrence is zero (for the case $n = 2$), the quantum state is separable, otherwise it is entangled.

As an example we consider the two-point Hubbard model (Steeb and Hardy, 2001). 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.

The two-point Hubbard model with cyclic boundary conditions is given by

$$\hat{H} = t(c_{1\uparrow}^\dagger c_{2\uparrow} + c_{1\downarrow}^\dagger c_{2\downarrow} + c_{2\uparrow}^\dagger c_{1\uparrow} + c_{2\downarrow}^\dagger c_{1\downarrow}) + U(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}) \tag{5}$$

where

$$n_{j\uparrow} := c_{j\uparrow}^\dagger c_{j\uparrow}, \qquad n_{j\downarrow} := c_{j\downarrow}^\dagger c_{j\downarrow}. \tag{6}$$

The Fermi operators $c_{j\uparrow}^\dagger, c_{j\downarrow}^\dagger, c_{j\uparrow}, c_{j\downarrow}$ obey the anticommutation relations

$$[c_{j,\sigma}^\dagger, c_{k,\sigma'}]_+ = \delta_{\sigma\sigma'}\delta_{jk} I, \qquad [c_{j,\sigma}^\dagger, c_{k,\sigma'}^\dagger]_+ = [c_{j,\sigma}, c_{k,\sigma'}]_+ = 0. \tag{7}$$

$\hat{H}$ commutes with the total number operator $\hat{N}$, and the total spin operator $\hat{S}_z$ in the z direction

$$\hat{N} := \sum_{j=1}^{2}(c_{j\uparrow}^{\dagger}c_{j\uparrow} + c_{j\downarrow}^{\dagger}c_{j\downarrow}) \tag{8}$$

$$\hat{S}_z := \frac{1}{2}\sum_{j=1}^{2}(c_{j\uparrow}^{\dagger}c_{j\uparrow} - c_{j\downarrow}^{\dagger}c_{j\downarrow}). \tag{9}$$

We consider the subspace with two electrons, $N = 2$ and $S_z = 0$. A basis for 2 particles with total spin 0 is

$$|s_1\rangle := c_{1\uparrow}^{\dagger}c_{1\downarrow}^{\dagger}|0\rangle, \qquad |s_2\rangle := c_{1\uparrow}^{\dagger}c_{2\downarrow}^{\dagger}|0\rangle, \qquad |s_3\rangle := c_{2\uparrow}^{\dagger}c_{1\downarrow}^{\dagger}|0\rangle, \qquad |s_4\rangle := c_{2\uparrow}^{\dagger}c_{2\downarrow}^{\dagger}|0\rangle \tag{10}$$

where $\langle 0|0\rangle = 1$. Applying $\hat{H}$ to the basis gives

$$\hat{H}|s_1\rangle = t|s_2\rangle + t|s_3\rangle + U|s_1\rangle \tag{11}$$

$$\hat{H}|s_2\rangle = t|s_1\rangle + t|s_4\rangle \tag{12}$$

$$\hat{H}|s_3\rangle = t|s_1\rangle + t|s_4\rangle \tag{13}$$

$$\hat{H}|s_4\rangle = t|s_2\rangle + t|s_3\rangle + U|s_4\rangle. \tag{14}$$

Identifying $|s_i\rangle$ with elements $\mathbf{e}_i$ of the standard basis in $\mathbf{C}^4$ yields the matrix representation of $\hat{H}$

$$\hat{H} = \begin{pmatrix} U & t & t & 0 \\ t & 0 & 0 & t \\ t & 0 & 0 & t \\ 0 & t & t & U \end{pmatrix}. \tag{15}$$

Suppose a Hamilton operator $\hat{K}$ can be written as $\hat{K} = A_1 \otimes I_2 + I_2 \otimes A_2$ where $A_1, A_2 \in M^2$ and I_2 is the 2×2 identity matrix. Then we have (Steeb, 1997)

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

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 matrix representation of $\hat{H}$, however we have

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

The diagonal matrix diag$(U, 0, 0, U)$ cannot be written in the form $A_1 \otimes I_2 + I_2 \otimes A_2$. Thus we conclude that almost all initial separable states evolve into entangled states under the time evolution of the model.

The eigenvalues of $\hat{H}$ are $E_1 = 0$, $E_2 = U$, $E_{3,4} = \frac{1}{2}(U \pm \sqrt{U^2 + 16t^2})$.

For all U and t the Hamilton operator $\hat{H}$ can be written as (spectral representation)

$$\hat{H} = \sum_{j=1}^{4} E_j |x_j\rangle\langle x_j| \tag{16}$$

where E_j are the eigenvalues and $|x_j\rangle$ are the corresponding orthonormal eigenstates of $\hat{H}$.

To find the time evolution for the two-point Hubbard model we solve the Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial \tau} = \hat{H}\psi.$$

Thus

$$|\psi(\tau)\rangle = U_{\hat{H}}(\tau)|\psi(0)\rangle \tag{17}$$

where $|\psi(0)\rangle$ is the initial state and

$$U_{\hat{H}}(\tau) := e^{-i\hat{H}\tau/\hbar}. \tag{18}$$

For $t = 0$, the unitary transformation $U_{\hat{H}}(\tau)$ implements a phase change.

For the initial state $|s_1\rangle$ we find the condition for separability for $U_{\hat{H}}(\tau)|s_1\rangle$ is

$$UE_3 m^4 \left(E_4 \exp\left(\frac{i\tau}{2\hbar}(E_4 - E_3)\right) - E_3 \exp\left(\frac{i\tau}{2\hbar}(E_3 - E_4)\right)\right)^2 = \frac{1}{4}\exp\left(-i\frac{\tau}{\hbar}U\right) \tag{19}$$

where

$$m := \frac{1}{\sqrt{2}}((E_3 - U)^2 + 4t^2)^{-\frac{1}{2}}.$$

To satisfy the imaginary part of Eq. (19) we find the condition

$$E_4 \sin\left(\frac{\tau}{\hbar}E_4\right) - E_3 \sin\left(\frac{\tau}{\hbar}E_3\right) = 0.$$

Thus we find $U_{\hat{H}}(\tau)|s_1\rangle$ is entangled when the condition is not satisfied.

For the initial state $|s_2(\tau)\rangle$ we find the condition for separability for $U_{\hat{H}}(\tau)|s_2\rangle$ is

$$UE_4^{-1} m^4 \exp\left(-i\frac{\tau}{\hbar}U\right)\left(E_4^2 \exp\left(\frac{i\tau}{2\hbar}(E_4 - E_3)\right) - E_3^2 \exp\left(\frac{i\tau}{2\hbar}(E_3 - E_4)\right)\right)^2 = \frac{1}{4}. \tag{20}$$

To satisfy the imaginary part of Eq. (20) we find the condition

$$E_4^2 \sin\left(\frac{\tau}{\hbar}E_3\right) - E_3^2 \sin\left(\frac{\tau}{\hbar}E_4\right) = 0.$$

Thus we find $U_{\hat{H}}(\tau)|s_2\rangle$ is entangled when the condition is not satisfied.

For $U_{\hat{H}}(\tau)|s_3\rangle$ (respectively $U_{\hat{H}}(\tau)|s_4\rangle$) we find the condition for separability is identical to that for $U_{\hat{H}}(\tau)|s_2\rangle$ (respectively $U_{\hat{H}}(\tau)|s_1\rangle$).

Next we determine the conditions that the states

$$|\Phi^+\rangle := \frac{1}{\sqrt{2}}(|s_1\rangle + |s_4\rangle), \qquad |\Phi^-\rangle := \frac{1}{\sqrt{2}}(|s_1\rangle - |s_4\rangle)$$

$$|\Psi^+\rangle := \frac{1}{\sqrt{2}}(|s_2\rangle + |s_3\rangle), \qquad |\Psi^-\rangle := \frac{1}{\sqrt{2}}(|s_2\rangle - |s_3\rangle)$$

are entangled under time evolution of the model. They are maximally entangled states. These are the Bell states and form a basis in $\mathbf{C}^4$.

For $U_{\hat{H}}(\tau)|\Phi^+\rangle$ we find the condition for separability

$$2UE_3m^4\left(E_4\exp\left(\frac{i\tau}{2\hbar}(E_4 - E_3)\right) - E_3\exp\left(\frac{i\tau}{2\hbar}(E_3 - E_4)\right)\right)^2 = 0. \quad (21)$$

Thus when $U_{\hat{H}}(\tau)|\Phi^+\rangle$ is not entangled $U_{\hat{H}}(\tau)|s_1\rangle$ and $U_{\hat{H}}(\tau)|s_4\rangle$ are entangled and vice versa. For $U \neq 0$ the condition becomes

$$E_4 = E_3\exp\left(i\frac{\tau}{\hbar}(E_3 - E_4)\right)$$

which has no real solutions for τ. Thus $U_{\hat{H}}(\tau)|\Phi^+\rangle$ is entangled for all τ.

For $U_{\hat{H}}(\tau)|\Phi^-\rangle$ we find the condition for separability

$$\exp\left(-2i\frac{\tau}{\hbar}U\right) = 0. \quad (22)$$

Of course, this equation cannot be satisfied. Thus $U_{\hat{H}}(\tau)|\Phi^-\rangle$ is entangled for all τ. For $U_{\hat{H}}(\tau)|\Psi^+\rangle$ we find the condition for separability

$$-2UE_4^{-1}m^4\left(E_4^2\exp\left(\frac{i\tau}{2\hbar}(E_4 - E_3)\right) - E_3^2\exp\left(\frac{i\tau}{2\hbar}(E_3 - E_4)\right)\right)^2 = 0. \quad (23)$$

Thus when $U_{\hat{H}}(\tau)|\Psi^+\rangle$ is not entangled $U_{\hat{H}}(\tau)|s_2\rangle$ and $U_{\hat{H}}(\tau)|s_3\rangle$ are entangled and vice versa. We find that $U_{\hat{H}}(\tau)|\Psi^+\rangle$ is entangled for all τ.

For $U_{\hat{H}}(\tau)|\Psi^-\rangle$ we find the condition for separability, $\frac{1}{2} = 0$, cannot be satisfied. Thus $U_{\hat{H}}(\tau)|\Psi^-\rangle$ is entangled for all τ.

The behavior described above can be understood if we realize that the Hubbard model admits a discrete symmetry under the change $1 \to 2, 2 \to 1$. Thus we have a finite group with two elements. We obtain two irreducible representation

(Steeb, 2003). The group-theoretical reduction leads to the invariant subspaces

$$S_1 = \left\{ |\psi_1\rangle = \frac{1}{\sqrt{2}}(c^\dagger_{1\downarrow} c^\dagger_{1\uparrow}|0\rangle + c^\dagger_{2\downarrow} c^\dagger_{2\uparrow}|0\rangle, \quad |\psi_2\rangle = \frac{1}{\sqrt{2}}(c^\dagger_{1\downarrow} c^\dagger_{2\uparrow}|0\rangle + c^\dagger_{2\downarrow} c^\dagger_{1\uparrow}|0\rangle) \right\}$$

$$S_2 = \left\{ |\psi_3\rangle = \frac{1}{\sqrt{2}}(c^\dagger_{1\downarrow} c^\dagger_{1\uparrow}|0\rangle - c^\dagger_{2\downarrow} c^\dagger_{2\uparrow}|0\rangle, \quad |\psi_4\rangle = \frac{1}{\sqrt{2}}(c^\dagger_{1\downarrow} c^\dagger_{2\uparrow}|0\rangle - c^\dagger_{2\downarrow} c^\dagger_{1\uparrow}|0\rangle) \right\}.$$

These four states can be considered as the Bell states. In the Bell basis the matrix representation of the Hubbard model is given by (where we use the ordering $|\Phi^+\rangle, |\Psi^+\rangle, |\Psi^-\rangle, |\Psi^-\rangle$)

$$\begin{pmatrix} U & 2t & 0 & 0 \\ 2t & 0 & 0 & 0 \\ 0 & 0 & U & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Thus the ground state is not a Bell state, but it is also not a separable state. We used a program to perform the symbolic calculations and most of the simplification of the separability conditions given above. The program makes use of SymbolicC++ (Shi *et al.*, 2000) to do the calculations and simplification. The Hubbard model can also be considered in Bloch representation. The entanglement can be considered in the momentum space. It is also worthwhile to consider entanglement of the two-dimensional Hubbard model with phonon coupling (Steeb *et al.*, 1986).

$$\hat{H} = t \sum_{\sigma \in \{\uparrow,\downarrow\}} (c^\dagger_{1\sigma} c_{2\sigma} + c^\dagger_{2\sigma} c_{1\sigma}) + U(n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} n_{2\downarrow})$$
$$+ \omega b^\dagger b + k \sum_{\sigma \in \{\uparrow,\downarrow\}} (c^\dagger_{1\sigma} c_{2\sigma} + c^\dagger_{2\sigma} c_{1\sigma})(b^\dagger + b)$$

where $b, b^\dagger$ are the Bose annihilation and creation operators for the vibrational mode, respectively. In this case we have a product space of the states given above and the number states $|n\rangle = (n!)^{-1/2}(b^\dagger)^n|0\rangle$ with $b|0\rangle = 0$, $\langle 0|0\rangle = 1$ and $n = 0, 1, 2, \ldots$. For $S'_z = 0$ the basis in the product space is now given as

$$S'_1 = \{|\psi_1\rangle \otimes |n\rangle, |\psi_2\rangle \otimes |n\rangle, \quad n = 0, 1, 2, \ldots\}$$
$$S'_2 = \{|\psi_3\rangle \otimes |n\rangle, \quad n = 0, 1, 2, \ldots\}$$
$$S'_3 = \{|\psi_4\rangle \otimes |n\rangle, \quad n = 0, 1, 2, \ldots\}$$

For the subspace S'_1 we obtain

$$\hat{H}|\psi_1\rangle \otimes |n\rangle = 2t|\psi_2\rangle \otimes |n\rangle + (U + n\omega)|\psi_1\rangle \otimes |n\rangle$$
$$+ 2k(n+1)^{1/2}|\psi_2\rangle \otimes |n+1\rangle + 2kn^{1/2}|\psi_2\rangle \otimes |n-1\rangle$$

$$\hat{H}|\psi_2\rangle \otimes |n\rangle = 2t|\psi_1\rangle \otimes |n\rangle + n\omega|\psi_2\rangle \otimes |n\rangle + 2k(n+1)^{1/2}|\psi_1\rangle \otimes |n+1\rangle + 2kn^{1/2}|\psi_1\rangle \otimes |n-1\rangle.$$

In the subspace S_2' we have the energy levels $U + n\omega$ $(n = 0, 1, 2\ldots)$ and in the subspace S_3' we find $n\omega$ $(n = 0, 1, 2, \ldots)$. In both cases the eigenvalues do not depend on k. This allows to study entanglement between Bose and Fermi states. For example, we could consider entangled states such as $\frac{1}{\sqrt{2}}(|\psi_1\rangle \otimes |0\rangle + |\psi_2\rangle \otimes |1\rangle)$.

REFERENCES

Hardy, Y. and Steeb, W.-H. (2001). *Classical and Quantum Computing with C++ and Java Simulations*, Birkhäuser, Basel, Switzerland.

Nielsen, M. A. and Chuang, I. L. (2000). *Quantum Computation and Quantum Information*, Cambridge University Press, Cambridge, UK.

Preskill, J. (2001). *Quantum Information and Computation*, Caltech, Pasadena, CA. http://www.theory.caltech.edu/~preskill/ph229

Shi, Tan Kiat, Steeb, W.-H., and Hardy, Y. (2000). *Symbolic C++: An Introduction to Computer Algebra Using Object-Oriented Programming*, Springer-Verlag, London.

Steeb, W.-H. (1997). *Matrix Calculus and Kronecker Product With Applications and C++ Programs*, World Scientific, Singapore.

Steeb, W.-H. (2003). *Problems and Solutions in Theoretical and Mathematical Physics*, World Scientific, Vol. II, Advanced Level, Singapore.

Steeb, W.-H. and Hardy, Y. (2000). *International Journal of Theoretical Physics* **39**, 2765.

Steeb, W.-H. and Hardy, Y. (2001). *International Journal of Modern Physics C* **12**, 235–245.

Steeb, W.-H. and Hardy, Y. (2002). *Zeitschrift für Naturforschung* **57a**, 400.

Steeb, W.-H. and Hardy, Y. (2004). *Problems and Solutions in Quantum Computing and Quantum Information*, World Scientific, Singapore.

Steeb, W.-H., Louw, J. A., Villet, C. M., and Kunick, A. (1986). *Physica Scripta* **34**, 245.

Wooters, W. K. (1998). *Physical Review Letters* **80**, 2245.