

Kronecker Products of Matrices and an Application to Fermi Systems

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An identity for the trace of an exponential function of Kronecker products of matrices is proved. This identity plays an important role for the calculation of the grand potential of interacting Fermi systems. For the Hamiltonian $H = \sum_i n_{i\uparrow} n_{i\downarrow}$, where $n_{i\sigma} = c_{i\sigma}^+ c_{i\sigma}$ ($c_{i\sigma}^+$: Fermi creation operator at the i th site with spin σ) we calculate the specific heat for different numbers of electrons per lattice site. Finally, we extend our calculations to find approximative solutions of the Hubbard model.

In the present paper we prove an identity concerning the trace of an exponential function of Kronecker products of matrices. Then we give an application to Fermi systems.

First of all let us introduce the notation. I denotes the $n \times n$ unit matrix. Let $X \otimes Y$ be the Kronecker product (tensor product) of the $n \times n$ matrices X and Y . $\text{tr } X$ denotes the trace of the $n \times n$ matrix X . Let $[X, Y]$ be the commutator (Lie bracket) of the $n \times n$ matrices X and Y . We notice that if $[X, Y] = 0$, then $\exp(X + Y) = \exp(X) \exp(Y)$, where $\exp(\cdot)$ denotes the exponential function.

Steeb and Wilhelm (1981) proved the following:

Theorem 1. Let A_1, A_2, B_1, B_2 be real $n \times n$ matrices. Then

$$\begin{aligned} \text{tr} \exp(A_1 \otimes I \otimes B_1 \otimes I + I \otimes A_2 \otimes I \otimes B_2) \\ \equiv (\text{tr} \exp(A_1 \otimes B_1)) (\text{tr} \exp(A_2 \otimes B_2)) \end{aligned} \quad (1)$$

An extension of the formula (1) is

Theorem 2. Let $A_1, A_2, \dots, A_N, B_1, B_2, \dots, B_N$ be real $n \times n$ matrices.

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Then

$$\begin{aligned}
 & \text{tr exp}(A_1 \otimes I \otimes \cdots \otimes I \otimes B_1 \otimes I \otimes \cdots \otimes I \\
 & \quad + I \otimes A_2 \otimes \cdots \otimes I \otimes I \otimes B_2 \otimes \cdots \otimes I \\
 & \quad \vdots \\
 & \quad + I \otimes I \otimes \cdots \otimes A_N \otimes I \otimes I \otimes \cdots \otimes B_N) \\
 & \equiv (\text{tr exp}(A_1 \otimes B_1))(\text{tr exp}(A_2 \otimes B_2)) \cdots (\text{tr exp}(A_N \otimes B_N)) \quad (2)
 \end{aligned}$$

The purpose of this paper is to give an extension of Theorem 1 and Theorem 2.

Theorem 3. Let A_1, A_2, B_1, B_2, C be real $n \times n$ matrices. Assume that

$$[A_1, C] = [A_2, C] = [B_1, C] = [B_2, C] = 0$$

Then

$$\begin{aligned}
 & \text{tr exp}(A_1 \otimes I \otimes B_1 \otimes I + I \otimes A_2 \otimes I \otimes B_2 + C \otimes I \otimes I \otimes I \\
 & \quad + I \otimes C \otimes I \otimes I + I \otimes I \otimes C \otimes I + I \otimes I \otimes I \otimes C) \\
 & \equiv (\text{tr exp}(A_1 \otimes B_1 + C \otimes I + I \otimes C))(\text{tr exp}(A_2 \otimes B_2 + C \otimes I + I \otimes C)) \quad (3)
 \end{aligned}$$

The proof is completely parallel to that of Theorem 1 (Steeb and Wilhelm, 1981), where we have taken into account that C commutes with A_1, A_2, B_1 , and B_2 .

An extension of formula (3) is as follows:

Theorem 4. Let $A_1, A_2, \dots, A_N, B_1, B_2, \dots, B_N, C$ be real $n \times n$ matrices. Assume that $[A_i, C] = [B_i, C] = 0$ for $i = 1, \dots, N$. Then

$$\begin{aligned}
 & \text{tr exp}(A_1 \otimes I \otimes \cdots \otimes I \otimes B_1 \otimes I \otimes \cdots \otimes I \\
 & \quad + I \otimes A_2 \otimes \cdots \otimes I \otimes I \otimes B_2 \otimes \cdots \otimes I \\
 & \quad \vdots \\
 & \quad + I \otimes I \otimes \cdots \otimes A_N \otimes I \otimes I \otimes \cdots \otimes B_N \\
 & \quad + C \otimes I \otimes \cdots \otimes I \otimes I \otimes I \otimes \cdots \otimes I \\
 & \quad + I \otimes C \otimes \cdots \otimes I \otimes I \otimes I \otimes \cdots \otimes I \\
 & \quad \vdots \\
 & \quad + I \otimes I \otimes \cdots \otimes I \otimes I \otimes I \otimes \cdots \otimes C) \\
 & = \prod_{i=1}^N \text{tr exp}(A_i \otimes B_i + C \otimes I + I \otimes C) \quad (4)
 \end{aligned}$$

Before we describe the connection with Fermi systems let us consider a special case of identity (4). Assume that $A_1 = \cdots = A_N = B_1 = \cdots = B_N$.

We put $A = A_1 = \dots = B_N$. Then the right-hand side of identity (4) takes the form

$$(\text{tr exp}(A \otimes A + C \otimes I + I \otimes C))^N \tag{5}$$

Since $[A, C] = 0$, it follows that

$$\begin{aligned} &(\text{tr exp}(A \otimes A + C \otimes I + I \otimes C))^N \\ &\equiv (\text{tr}(\text{exp}(A \otimes A) \text{exp}(C \otimes I) \text{exp}(I \otimes C)))^N \end{aligned} \tag{6}$$

Assume that the matrices A and C can be written as $A = \sqrt{a} X$, $C = bY$, where $a \in \mathbb{R}^+$, $b \in \mathbb{R}$ and $X^2 = X$, $Y^2 = Y$. This means that X and Y are idempotent. Then we obtain

$$\begin{aligned} &(\text{tr exp}(A \otimes A + C \otimes I + I \otimes C))^N \\ &\equiv (\text{tr}(I \otimes I + (e^a - 1)(X \otimes X))(I \otimes I + (e^b - 1)(Y \otimes I)) \\ &\quad \times (I \otimes I + (e^b - 1)(I \otimes Y)))^N \end{aligned} \tag{7}$$

Using the identity $(R \otimes S)(U \otimes V) \equiv (RU) \otimes (SV)$ it follows that

$$\begin{aligned} &(\text{tr exp}(A \otimes A + C \otimes I + I \otimes C))^N \\ &\equiv (\text{tr}(I \otimes I + (e^b - 1)(Y \otimes I + I \otimes Y) + (e^a - 1)(X \otimes X) \\ &\quad + (e^b - 1)^2(Y \otimes Y) + (e^a - 1)(e^b - 1)(XY \otimes X + X \otimes XY) \\ &\quad + (e^a - 1)(e^b - 1)^2(XY \otimes XY)))^N \end{aligned} \tag{8}$$

If we assume that I is the 2×2 unit matrix and

$$X = Y = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{9}$$

then

$$(\text{tr exp}(A \otimes A + C \otimes I + I \otimes C))^N \equiv (1 + 2e^b + e^{a+2b})^N \tag{10}$$

Let us now describe the connection with Fermi systems. Fermi creation operators with spin up and spin down, respectively, have the matrix representation [Steeb (1977)] ($i = 1, \dots, N$)

$$\begin{array}{c} \text{\textit{i}th place} \\ \downarrow \\ c_{i\uparrow}^+ = \underbrace{\sigma_z \otimes \dots \otimes \sigma_z \otimes (\frac{1}{2}\sigma_+) \otimes I \otimes \dots \otimes I}_{2N \text{ times}} \end{array} \tag{11}$$

$$\begin{array}{c} \text{\textit{(i+N)th} place} \\ \downarrow \\ c_{i\downarrow}^+ = \underbrace{\sigma_z \otimes \dots \otimes \sigma_z \otimes (\frac{1}{2}\sigma_+) \otimes I \otimes \dots \otimes I}_{2N \text{ times}} \end{array} \tag{12}$$

where I is the 2×2 unit matrix and

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma_+ = \begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix} \quad (13)$$

For the Fermi annihilation operators with spin up and down, respectively, we have to replace σ_+ by σ_- , where

$$\sigma_- = \begin{pmatrix} 0 & 0 \\ 2 & 0 \end{pmatrix} \quad (14)$$

Consider now the Hamilton operator

$$K = a \sum_{i=1}^N c_{i\uparrow}^+ c_{i\uparrow} c_{i\downarrow}^+ c_{i\downarrow} + b \sum_{i=1}^N (c_{i\uparrow}^+ c_{i\uparrow} + c_{i\downarrow}^+ c_{i\downarrow}) \quad (15)$$

where $a, b \in \mathbb{R}$. Since $\sigma_z^2 = I$ and

$$\left(\frac{1}{2}\sigma_+\right)\left(\frac{1}{2}\sigma_-\right) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad (16)$$

we obtain

$$c_{i\uparrow}^+ c_{i\uparrow} = I \otimes \cdots \otimes I \otimes \begin{matrix} \text{ith place} \\ | \\ \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \end{matrix} \otimes I \otimes \cdots \otimes I \quad (17)$$

$$c_{i\downarrow}^+ c_{i\downarrow} = I \otimes \cdots \otimes I \otimes \begin{matrix} \text{(i+N)th place} \\ | \\ \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \end{matrix} \otimes I \otimes \cdots \otimes I \quad (18)$$

and

$$c_{i\uparrow}^+ c_{i\uparrow} c_{i\downarrow}^+ c_{i\downarrow} = I \otimes \cdots \otimes I \otimes \begin{matrix} \text{ith place} \\ | \\ \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \end{matrix} \otimes I \otimes \cdots \otimes I \otimes \begin{matrix} \text{(i+N)th place} \\ | \\ \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \end{matrix} \otimes I \otimes \cdots \otimes I \quad (19)$$

Consequently, the problem to calculate $\text{tr exp}(K)$ has been solved above [equation (10)]. We mention that a Wick theorem for the Hamiltonian (15) has been derived by Steeb (1976).

Let us now give two applications. Thermodynamic properties of the Hubbard model

$$H = \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^+ c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (20)$$

have been investigated by several authors. However, in most cases only the half-filled case ($n_e = N_e/N = 1$, $N_e =$ number of electrons, $N =$ number of lattice sites) has been considered. In our first application we neglect the kinetic part. The resulting Hamiltonian

$$H = U \sum_{i=1}^N n_{i\uparrow} n_{i\downarrow} \tag{21}$$

can be viewed as a simple model for an insulator. For a different number of electrons per lattice site we calculate the thermodynamic quantities. In our second application we include the kinetic part.

For the Hamiltonian (21) the grand thermodynamic potential per lattice site is given by

$$\frac{\Omega}{N} = -\frac{1}{\beta} \ln(1 + 2 e^{\beta\mu} + e^{\beta(2\mu-U)}) \tag{22}$$

where μ is the chemical potential. For the number of electrons per lattice site n_e we find

$$n_e = \frac{2(e^{\beta\mu} + e^{\beta(2\mu-U)})}{1 + 2e^{\beta\mu} + e^{\beta(2\mu-U)}} \tag{23}$$

where $0 \leq n_e \leq 2$. Because of the Pauli principle $\mu \rightarrow \infty$ as $n_e \rightarrow 2$. In the following we consider the range $0 < n_e < 2$. Furthermore we introduce the dimensionless quantities $\tilde{\mu} = \mu/U$ and $\tilde{\beta} = \beta U$ (or $\tilde{T} = kT/U$). Equation (23) can be inverted to yield the chemical potential

$$\tilde{\mu} = 1 + \tilde{\beta}^{-1} \ln \left\{ \frac{(n_e - 1) + [(n_e - 1)^2 + n_e(2 - n_e) e^{-\tilde{\beta}}]^{1/2}}{2 - n_e} \right\} \tag{24}$$

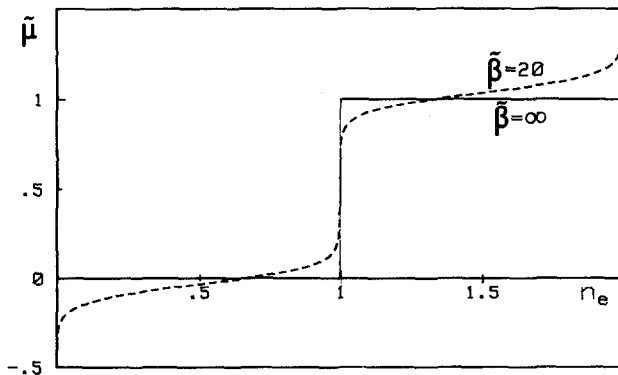


Fig. 1. Dimensionless chemical potential as a function of n_e for $\tilde{\beta} = 20$ and $\tilde{\beta} = \infty$.

At $n_e = 1$ we find $\tilde{\mu} = 1/2$ for all temperatures. In Figure 1 the chemical potential $\tilde{\mu}$ is plotted as a function of n_e for $\tilde{T} = 0$ and $\tilde{\beta} = 20$. For $\tilde{\beta} \rightarrow \infty$ ($\tilde{T} \rightarrow 0$) we find a step function. For $0 < n_e < 1$ the chemical potential $\tilde{\mu}$ is equal to 0. For $1 < n_e < 2$ the chemical potential is equal to 1. For $\tilde{\beta} = 20$ we see that the function $\tilde{\mu}(n_e)$ is approximately a step function. Let $U = 1$ eV and $\tilde{\beta} = 20$; then $T = 580$ K. From the Helmholtz free energy $F = \Omega + \mu N_e$, we obtain the dimensionless entropy per lattice site

$$\tilde{S} = \ln z - \beta(2\tilde{\mu} e^{\tilde{\beta}\tilde{\mu}} + (2\tilde{\mu} - 1) e^{\tilde{\beta}(2\tilde{\mu}-1)})z^{-1} \quad (25)$$

where $\tilde{S} = S/Nk$ and

$$z = 1 + 2 e^{\tilde{\beta}\tilde{\mu}} + e^{\tilde{\beta}(2\tilde{\mu}-1)} \quad (26)$$

For the dimensionless specific heat per lattice site we find

$$\tilde{C}_v = \tilde{\beta}[(g+1)(n_e x^{-1} - 2g e^{\tilde{\beta}})z^{-1} + n_e(2gx - n_e e^{-\tilde{\beta}})(2gx)^{-1}] + \tilde{\beta}^2 g(n_e x^{-1} - g(1 - n_e x^{-1}) e^{\tilde{\beta}})z^{-2} \quad (27)$$

where $\tilde{C}_v = C_v/Nk_B$,

$$g = [(n_e - 1) + x](2 - n_e)^{-1} \quad (28)$$

and

$$x = [(n_e - 1)^2 + n_e(2 - n_e) e^{-\tilde{\beta}}]^{1/2} \quad (29)$$

In Figure 2 we have plotted the dimensionless specific heat per lattice site \tilde{C}_v as a function of the dimensionless temperature \tilde{T} for different values of n_e , namely, $n_e = 0.5, 0.9, 1, 1.1, 1.5$. At low temperature \tilde{T} we have

$$\tilde{C}_v = \begin{cases} \frac{1}{8}\tilde{\beta}^2 e^{-\tilde{\beta}}, & \text{for } n_e = 0.5, 1.5 \\ \frac{1}{4}\tilde{\beta}^2 e^{-\tilde{\beta}/2}, & \text{for } n_e = 1 \end{cases} \quad (30)$$

We see that there is no power law of the form $\tilde{C}_v \sim \tilde{T}^\gamma$. Notice that the specific heat for a Fermi gas at low temperature is linear in the temperature.

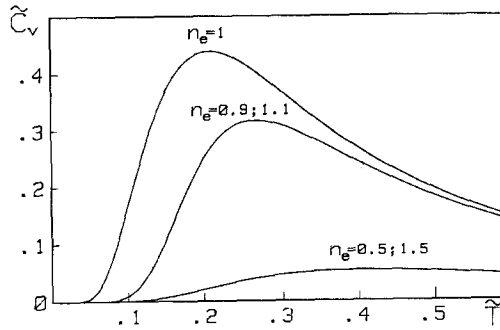


Fig. 2. Dimensionless heat capacity \tilde{C}_v as a function of the dimensionless temperature \tilde{T} for $n_e = 1, 1.1, 0.9, 1.5, 0.5$.

In the range $0 \leq \tilde{T} \leq 0.05$ the specific heat \tilde{C}_v is approximatively equal to zero. Let $U = 1$ eV then the temperature T related to $\tilde{T} = 0.05$ is $T = 580$ K. Furthermore the specific heat depends strongly on the number of electrons per lattice site. For $n_e = 1$ the heat capacity takes the maximal values. At $\tilde{T} = 0.2$ we have $\tilde{C}_v = 0.45$. Since $\tilde{C}_v = C_v / Nk_B$ we obtain $C_v = 3.74$ J/mol deg. At $n_e = 0.5$ the number of electrons is too small in order contribute significantly to the heat capacity. For $n_e = 1.5$ we find the same result. At first sight this result is surprising. The reason is that the Pauli principle comes into play. No more than two electrons can be placed at each lattice site.

Let us now briefly describe how we can include the kinetic part. It is known that the Hubbard model can only be solved (i.e., the ground state energy can be calculated) for the linear chain with cyclic boundary conditions in the half-filled case. Thus we use a variational principle to find an upper bound for the grand thermodynamic potential. This can be done since the Hubbard model is bounded from below. For itinerant electron models for describing ferromagnetism or antiferromagnetism in most cases we have $U \gg t$. Consequently, the kinetic part can be treated as a perturbation.

The grand canonical density matrix, W_0 , for a system with Hamiltonian H and number operator N_e at temperature $1/\beta$ and chemical potential μ can be derived by specifying it to be that which minimizes the grand thermodynamic potential

$$\Omega = \text{Tr } W(H - \mu N_e) + \frac{1}{\beta} \text{Tr}(W \ln W)$$

over all W . W is a linear, Hermitian Hilbert-Schmidt operator with unit trace. The condition that the first functional derivative vanishes leads uniquely to

$$W_0 = \frac{\exp[-\beta(H - \mu N_e)]}{\text{Tr}\{\exp[-\beta(H - \mu N_e)]\}}$$

The fact that W_0 gives a minimum follows from the form of the second functional derivative at $W = W_0$. This operator is positive definite since W_0 is positive definite.

Now we start with

$$W_t = \frac{\exp\left(-\lambda_1 \sum_n \bar{c}_{n\uparrow}^+ \bar{c}_{n\uparrow} \bar{c}_{n\downarrow}^+ \bar{c}_{n\downarrow} - \lambda_2 \sum_n \bar{c}_{n\uparrow}^+ \bar{c}_{n\uparrow} - \lambda_3 \sum_n \bar{c}_{n\downarrow}^+ \bar{c}_{n\downarrow}\right)}{\text{Tr}\left[\exp\left(-\lambda_1 \sum_n \bar{c}_{n\uparrow}^+ \bar{c}_{n\uparrow} \bar{c}_{n\downarrow}^+ \bar{c}_{n\downarrow} - \lambda_2 \sum_n \bar{c}_{n\uparrow}^+ \bar{c}_{n\uparrow} - \lambda_3 \sum_n \bar{c}_{n\downarrow}^+ \bar{c}_{n\downarrow}\right)\right]} \quad (31)$$

where n runs over all lattice sites. The operators \bar{c}^+ , \bar{c} , and c^+ , c are connected by

$$A = e^{iS} \bar{A} e^{-iS} \quad (32)$$

where S is the Hermitian operator

$$S = i \sum_{mn} \left(\frac{\phi_{m-n}}{2} \bar{c}_{n\uparrow} \bar{c}_{m\downarrow} e^{iQR_m} - \frac{\phi_{m-n}}{2} \bar{c}_{m\uparrow} \bar{c}_{n\downarrow} e^{-iQR_m} \right) \quad (33)$$

The variational parameters are λ_1 , λ_2 , λ_3 , Q , and ϕ_{n-m} . The operator S is the Fourier transform of

$$S = i \sum_k \left(\frac{\alpha_k}{2} \bar{c}_{k\uparrow}^+ \bar{c}_{k+Q\downarrow} - \frac{\alpha_k}{2} \bar{c}_{k+Q\downarrow}^+ \bar{c}_{k\uparrow} \right) \quad (34)$$

where $c_{k\sigma}^+$ and $c_{k\sigma}$ are the Fermi operators in Bloch representation. This means we assume cyclic boundary conditions. For practical calculations we perform the unitary transformation in the k space. Then with the help of the Fourier transform we calculate the rotated Hamiltonian in the Wannier representation. Finally we perform our trace calculation with the theorems given above.

When we would like to study the case with $t > U$ the starting point can be the trial density matrix

$$W_t = \frac{\exp \left\{ -\beta \sum_k [E_1(k) \bar{c}_{k\uparrow}^+ \bar{c}_{k\uparrow} + E_2(k) \bar{c}_{k\downarrow}^+ \bar{c}_{k\downarrow}] \right\}}{\text{Tr} \exp \left\{ -\beta \sum_k [E_1(k) \bar{c}_{k\uparrow}^+ \bar{c}_{k\uparrow} + E_2(k) \bar{c}_{k\downarrow}^+ \bar{c}_{k\downarrow}] \right\}} \quad (35)$$

together with the unitary transformation given by equations (32) and (34). The variational parameters are $\alpha_{k\sigma}$, $E_1(k)$, $E_2(k)$, and Q .

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