Question

第四章作业-itebd（选做，26分）

编写程序：

用ITEBD计算自旋为1的一维无限长Heisenberg模型的波函数并估算基态能量。奇异值分解可以调用cpplapack中的函数gesvd(…)或者你熟悉的函数.

1.

BLASINT gesvd(const char &jobu, const char &jobvt, const BLASINT &m, const BLASINT &n, Complex* matrix, const BLASINT &lda, double* s, Complex* u, const BLASINT &ldu, Complex* vt, const BLASINT &ldvt, Complex* work, const BLASINT &lwork, double* rwork, BLASINT &info);

matrix = u s vt

a) jobu, jobvt 取为 ‘A’；

b) m, n 为需要分解的矩阵 matrix 的行和列；

c) lda, ldu, ldvt可以简单看作相应矩阵的列；

d) work, rwork是额外需要的内存，具体大小参见 lapack手册 zgesvd, dgesvd.

第四章作业（选做，26分）

2.

```
Complex* A = new Complex[D*d*D];
Complex* B = new Complex[D*d*D];
```

3. 基态能量的估算

$$e^{-\tau h}|\psi\rangle \approx \alpha|\psi\rangle \approx e^{-\tau E_0}|\psi\rangle.$$

分析

我们先介绍一下“Imaginary Time-evolving Block Decimation”（ITEBD）。

就我理解，这是一种基于“power method”的一种求解矩阵最小本征值（也就是基态）的一种方法。通过“虚时演化+归一化“的方式将系统的状态还原到基态。

下面我们将具体来讲述该算法的基本原理：

1. 波函数的含时演化

在薛定谔绘景下，t 系统时刻的状态波函数可以表示为（初始时刻记为时间零点）：

$$|\Psi_t\rangle = \exp(-iHt)\,|\Psi_0\rangle$$

虚时情况下：

$$|\Psi_\tau\rangle = \frac{\exp(-H\tau)\,|\Psi_0\rangle}{\|\exp(-H\tau)\,|\Psi_0\rangle\,\|}$$

如果了解“power method”，那么应该可以看出虚时情况下的公式就是我们用来求解矩阵最小本征值的式子。

2. Power Method

对于厄米矩阵$H \in \mathbb{C}^{n*n}$，其最大本征值及相应的本征向量可以由下面的推导给出：

设H的本征值为$\lambda_1, \lambda_2, \ldots, \lambda_n$，对应的本征矢为$\nu_1, \nu_2, \ldots, \nu_n$，且$|\lambda_1| > |\lambda_2| > \cdots > |\lambda_n|$。

$\mathbb{C}^n$中的向量$\mathbf{x_0}$可以写为$\mathbf{x_0} = c_1\nu_1 + c_2\nu_2 + \cdots + c_n\nu_n$。（这是由厄米矩阵的本征空间是完备的决定的）

因此，我们有：

$$
\begin{aligned}
\mathbf{x_1} = H\mathbf{x_0} &= c_1\lambda_1\nu_1 + \cdots + c_n\lambda_n\nu_n \\
&\cdots \\
\mathbf{x_k} = H^k\mathbf{x_0} &= c_1\lambda_1^k\nu_1 + \cdots + c_n\lambda_n^k\nu_n \\
&= \lambda_1^k\left[c_1\nu_1 + c_2\left(\frac{\lambda_2}{\lambda_1}\right)^k\nu_2 + \cdots + c_n\left(\frac{\lambda_n}{\lambda_1}\right)^k\nu_n\right]
\end{aligned}
$$

当$k \to \infty$时，只会剩下ν_1项，但是由于λ_1^k会趋向于无穷大或无穷小；因此，每次迭代都需要将$\mathbf{x}$归一化。

上面时一般的“power method”，只能求解绝对值最大的特征值和对应的特征向量。下面我们将介绍求解最小特征值及对应特征向量的方法。

还是上面的矩阵，只不过$\lambda_1 < \lambda_2 < \cdots < \lambda_n$。

则：

$$\mathbf{x} = e^{-\beta H}\mathbf{x_0} = c_1e^{-\beta\lambda_1}\nu_1 + \cdots + c_ne^{-\beta\lambda_n}\nu_n$$

当$\beta \to \infty, \mathbf{x} \to \nu_1$。

这就是我们上面给出的虚时演化波函数的式子。实际计算中，一般$\tau \backsim 0.01$，也可能和λ_1相关。

3. Matrix Product State

基于奇异值分解我们可以将系统的状态用多个矩阵乘积的形式表示[1]：

> SVD guarantees for an arbitrary (rectangular) matrix M of dimensions $(N_A \times N_B)$ the existence of a decomposition:
>
> $$M = USV^\dagger,$$
>
> where
>
> - U is of dimension $(N_A \times \min(N_A, N_B))$ and has orthonormal columns (the **left singular vectors**), i.e. $U^\dagger U = I$; if $N_A \leq N_B$ this implies that it is unitary, and also $UU^\dagger = I$.
> - S is of dimension $(\min(N_A, N_B) \times \min(N_A, N_B))$, diagonal with non-negative entries $S_{aa} \equiv s_a$. These are the so-called **singular values**. The

number r of non-zero singular values is the **(Schmidt) rank** of M. In the following, we assume descending order: $s_1 \geq s_2 \geq \ldots \geq s_r > 0$.

- $V^\dagger$ is of dimension $\left(\min(N_A, N_B) \times N_B\right)$ and has orthonormal rows (the **right singular vectors**), i.e. $V^\dagger V = I$. If $N_A \geq N_B$ this implies that it is unitary, and also $VV^\dagger = I$.

Consider a lattice of L sites with d-dimensional local state spaces $\{\sigma_i\}$ on sites $i = 1, \ldots, L$. In fact, while we will be naturally thinking of a one-dimensional lattice, the following also holds for a lattice of arbitrary dimension on which sites have been numbered; however, MPS generated from states on higher-dimensional lattices will not be manageable in numerical practice. The most general pure quantum state on the lattice reads

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} c_{\sigma_1\ldots\sigma_L} |\sigma_1, \ldots, \sigma_L\rangle ,$$

where we have exponentially many coefficients $c_{\sigma_1\ldots\sigma_L}$ with quite oblique content in typical quantum many-body problems. Let us assume that it is normalized. Can we find a notation that gives a more local notion of the state (while preserving the quantum non-locality of the state)? Indeed, SVD allows us to do just that. The result may look quite forbidding, but will be shown to relate profoundly to familiar concepts of quantum physics. There are three ways of doing this that are of relevance to us.

Left-canonical matrix product state. In a first step, we **reshape** the state vector with d^L components into a matrix Ψ of dimension $\left(d \times d^{L-1}\right)$, where the coefficients are related as

$$\Psi_{\sigma_1,(\sigma_2\ldots\sigma_L)} = c_{\sigma_1\ldots\sigma_L}.$$

An SVD of Ψ gives

$$c_{\sigma_1\ldots\sigma_L} = \Psi_{\sigma_1,(\sigma_2\ldots\sigma_L)} = \sum_{a_1}^{r_1} U_{\sigma_1,a_1} S_{a_1,a_1} (V^\dagger)_{a_1,(\sigma_2\ldots\sigma_L)} \equiv \sum_{a_1}^{r_1} U_{\sigma_1,a_1} c_{a_1\sigma_2\ldots\sigma_L},$$

where in the last equality S and $V^\dagger$ have been multiplied and the resulting matrix has been reshaped back into a vector. The rank is $r_1 \leq d$. We now decompose the matrix U into a collection of d row vectors A^{σ_1} with entries $A^{\sigma_1}_{a_1} = U_{\sigma_1,a_1}$. At the same time, we reshape $c_{a_1\sigma_2\ldots\sigma_L}$ into a matrix $\Psi_{(a_1\sigma_2),(\sigma_3\ldots\sigma_L)}$ of dimension $\left(r_1 d \times d^{L-2}\right)$, to give

$$c_{\sigma_1 \ldots \sigma_L} = \sum_{a_1}^{r_1} A^{\sigma_1}_{a_1} \Psi_{(a_1 \sigma_2),(\sigma_3 \ldots \sigma_L)}.$$

Ψ is subjected to an SVD, and we have

$$\begin{aligned} c_{\sigma_1 \ldots \sigma_L} &= \sum_{a_1}^{r_1} \sum_{a_2}^{r_2} A^{\sigma_1}_{a_1} U_{(a_1 \sigma_2),a_2} S_{a_2,a_2} (V^\dagger)_{a_2,(\sigma_3 \ldots \sigma_L)} \\ &= \sum_{a_1}^{r_1} \sum_{a_2}^{r_2} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1,a_2} \Psi_{(a_2 \sigma_3),(\sigma_4 \ldots \sigma_L)}, \end{aligned}$$

where we have replaced U by a set of d matrices A^{σ_2} of dimension $(r_1 \times r_2)$ with entries $A^{\sigma_2}_{a_1,a_2} = U_{(a_1 \sigma_2),a_2}$ and multiplied S and $V^\dagger$, to be reshaped into a matrix Ψ of dimension $(r_2 d \times d^{L-3})$, where $r_2 \leq r_1 d \leq d^2$. Upon further SVDs, we obtain

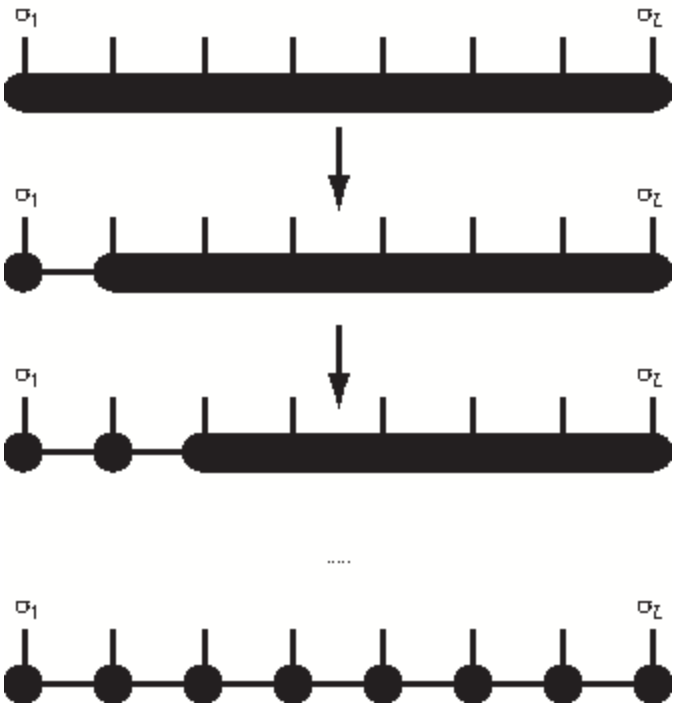
$$c_{\sigma_1 \ldots \sigma_L} = \sum_{a_1, \ldots, a_{L-1}} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1,a_2} \ldots A^{\sigma_{L_1}}_{a_{L-2},a_{L-1}} A^{\sigma_L}_{a_{L-1}}$$

or more compactly

$$c_{\sigma_1 \ldots \sigma_L} = A^{\sigma_1} A^{\sigma_2} \ldots A^{\sigma_{L-1}} A^{\sigma_L},$$

where we have recognized the sums over a_1, a_2 and so forth as matrix multiplications. The last set of matrices A^{σ_L} in fact consists of column vectors. If we wish, dummy indices 1 may be introduced in the first and last A to turn them into matrices, too. In any case, the (arbitrary) quantum state is now represented exactly in the form of a **matrix product state:**

$$|\psi\rangle = \sum_{\sigma_1, \ldots, \sigma_L} A^{\sigma_1} A^{\sigma_2} \ldots A^{\sigma_{L-1}} A^{\sigma_L} |\sigma_1, \ldots, \sigma_L\rangle .$$



Graphical representation of an iterative construction of an exact MPS representation of an arbitrary quantum state by a sequence of singular value decompositions.

---

1. Schollwöck, U. (2011). The density-matrix renormalization group in the age of matrix product states. Annals of Physics, 326(1), 96–192. https://doi.org/10.1016/j.aop.2010.09.012
pdf ↩