Physics 651: Assignment 1

(to be submitted by Tuesday, September 6, 2022)

1. Given a set of $2N$ Grassman numbers $\{\theta_1, \theta_2, \ldots, \theta_N, \eta_1, \eta_2, \ldots, \eta_N\}$, we would like to evaluate integrals of the form

$$\int d\theta\, d\eta\, e^{-\theta^T A \eta} = \int d\theta_1 \cdots d\theta_N\, d\eta_1 \cdots d\eta_N\, \exp\biggl(-\sum_{i,j} \theta_i A_{i,j} \eta_j\biggr),$$

where the indices i, j in the sum run over $1, 2, \ldots, N$. We can think of A as an $N \times N$ matrix of real- or complex-valued elements.

(a) For the $N = 2$ case, show explicitly that the integration yields $A_{1,1}A_{2,2} - A_{1,2}A_{2,1}$.

(b) Evaluate the integral expression for $N = 3$.

(c) Argue convincingly (in words, no explicit calculation is required) that the generic result is just $\det A$.

(d) Since the Grassman variables obey an "exlcusion principle" (viz., $\theta_i^2 = \eta_i^2 = 0$), we can think of them as describing fermionic degrees of freedom. The many-body wave function for a system of N (spinless) fermions is $\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N) = (N!)^{-1/2} \det A$, where $A_{i,j} = \psi_j(\boldsymbol{r}_i)$ is the single-particle wave function for the ith particle in the jth level. Return to the $N = 2$ case, and consider what happens (i) if $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ take arbitrary values but $\psi_1 = \psi_2$; and (ii) if $\psi_1 \neq \psi_2$ but $\boldsymbol{r}_1 = \boldsymbol{r}_2$. Explain what your mathematical observations mean physically.

2. A ball tossed into the air travels according to $h = v_0 t - \frac{1}{2} g t^2$. Here, v_0 is the initial vertical velocity (upward), and g is the gravitational acceleration (downward). A set of poorly taken measurements (eyeballed by an observer with a stopwatch against rough height marks on the wall) is given in the table below.

time t (s)	height h (m)
0.5	9.0
1.0	15.4
1.5	19.3
2.0	20.7
2.5	19.7
3.0	16.0
3.5	10.1
4.0	2.1

(a) Write out the corresponding linear system of eight equations and two unknowns in matrix format.

(b) Construct the Moore-Penrose pseudoinverse.

(c) Give best estimates (in the least squares sense) of the initial velocity (v_0) and the gravitational acceleration (g).

(d) The observer has reported no uncertainties on the measurements. How could you estimate the "error bars" on v_0 and g based on the data you were given? (One possibility is so-called Jackknife resampling.)

You may want to check your answer in Mathematica. To install the software, search for "Research Software" in MyOleMiss and follow the links. Open a new session (*File > New > Notebook*) from the menu bar. Type the following commands, each followed by *shift+return* or *shift+enter*.

```
tlist = {0.5, 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0}
hlist = {9.0, 15.4, 19.3, 20.7, 19.7, 16.0, 10.1, 2.1}
```

```
x[t_] = v0*t - (g/2)*t^2
xlist = Map[x, tlist]
row1 = xlist /. {v0 -> 1, g -> 0}
row2 = xlist /. {v0 -> 0, g -> 1}
MT = {row1, row2}
M = Transpose[MT]
M // MatrixForm
M.{v0, g} == xlist
hlist // MatrixForm
PseudoInverse[M] // MatrixForm
PseudoInverse[M].hlist
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3. The Pauli matrices are generators of the SU(2) algebra that governs spin-half quantum angular momenta. They are defined as

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Here, i is the imaginary number satisfying $i^2 = -1$.

(a) Compute the trace and determinant of each Pauli matrix.

(b) Show that $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = -i\sigma_x\sigma_y\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I$ (the identity matrix)

(c) Prove the anticommutation rule

$$\{\sigma_a, \sigma_b\} = \sigma_a\sigma_b + \sigma_b\sigma_a = 2I\delta_{a,b}.$$

Here, a and b range over the indices x, y, z, and δ is the Kronecker delta symbol.

(d) Prove the commutation rule

$$[\sigma_a, \sigma_b] = \sigma_a\sigma_b - \sigma_b\sigma_a = 2i\epsilon_{a,b,c}\sigma_c.$$

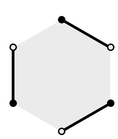
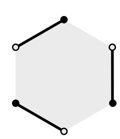
It is understood that the repeated c implies a summation over x, y, z, and ϵ is the Levi-Civita symbol.

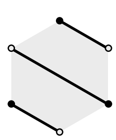
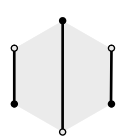
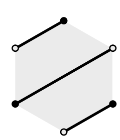
(e) We'll let $\boldsymbol{n}$ represent an arbitrary vector in $\mathbb{R}^3$ and adopt the notation $\boldsymbol{\sigma}$ (boldface sigma) to represent the Cartesian triple of matrices $(\sigma_x, \sigma_y, \sigma_z)$. Prove that

$$e^{i\boldsymbol{n}\cdot\boldsymbol{\sigma}} = I\cos\theta + i(\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma})\sin\theta,$$

where $\theta = |\boldsymbol{n}|$ and $\hat{\boldsymbol{n}} = \boldsymbol{n}/\theta$ is a unit vector. The easiest approach is to make use of the standard Taylor series expansions for the exponential, cosine, and sine functions.

4. Consider the following five configurations in which six sites (alternately coloured black and white around the hexagon) are grouped into oppositely coloured pairs:

$|1\rangle =$  $|2\rangle =$ 

$|3\rangle =$  $|4\rangle =$  $|5\rangle =$ 

(This is a reasonable basis choice for the valence electrons in a benenze ring; in that case, each bond represents an entangled pair of the form $(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$.) The overlap S is the matrix whose elements are the inner products $S_{i,j} = \langle i|j\rangle = 2^{L_{i,j}-3}$. The values are controlled by the number ($L_{i,j}$) of closed loops that are formed when configurations $|i\rangle$ and $|j\rangle$ are superimposed.

(a) Determine the matrix S, its trace ($\operatorname{tr} S$), determinant ($\det S$), and inverse (S^{-1}). Feel free to use a computer.

(b) This basis is not orthonormal. Show that the resolution of unity is $\hat{\mathbb{1}} = \sum_{i,j} |i\rangle S^{-1}_{i,j} \langle j|$. Specifically, prove (i) that $\hat{\mathbb{1}}|k\rangle = |k\rangle$ for each of $k = 1, 2, 3, 4, 5$ and (ii) that $\hat{\mathbb{1}}^2 = \hat{\mathbb{1}}$.

(c) The pairing rule actually supports $3! = 6$ possible configurations. (i) Draw the missing sixth state, call it $|6\rangle$, and argue that it is extraneous. (ii) Carry out the projection step $|6'\rangle = \hat{\mathbb{1}}|6\rangle$ to resolve $|6\rangle$ as a linear combination of the other five states. (iii) Check that $\langle 6|6'\rangle = \langle 6|\hat{\mathbb{1}}|6\rangle = 1$ to verify that no weight has been lost.

(d) Show that orthogonalization of this basis amounts to finding a matrix M that satisfies $M^T M = S$. This is the so-called "square root" of the matrix S. In general, this decomposition is not unique.

(e) Take as a starting point two states

$$|u_1\rangle = \sqrt{\frac{2}{5}}\big(|1\rangle + |2\rangle\big) \quad \text{and} \quad |u_2\rangle = \sqrt{\frac{2}{3}}\big(|1\rangle - |2\rangle\big)$$

that have been constructed to satisfy $\langle u_1|u_1\rangle = \langle u_2|u_2\rangle = 1$ and $\langle u_1|u_2\rangle = 0$. Perform one step in the Gram-Schmidt process to generate the next state,

$$|u_3\rangle = -\frac{2}{\sqrt{15}}\big(|1\rangle + |2\rangle\big) + \sqrt{\frac{5}{3}}|3\rangle.$$

Confirm that $\{|u_1\rangle, |u_2\rangle, |u_3\rangle\}$ constitute an orthonormal (sub)set. In principle, you could continue with further Gram-Schmidt steps to generate $|u_4\rangle$ and $|u_5\rangle$, but please don't!

I encourage you to make your life easier by seeking computer assistance for part (a). You'll want to determine the loop counts by hand, but everything else can be automated. Here (with some entries elided) is the relevant code in Mathematica:

```
L = {{3, 1, 2, 2, 2}, {1, 3, 2, 2, 2}, ..., {2, 2, 1, 1, 3}}
S = Map[((1/2)^(3 - #)) &, L]
S // MatrixForm
Tr[S]
Det[S]
Sinv = Inverse[S]
Sinv // MatrixForm
```