Physics 651: Assignment 2

(to be submitted by Thursday, September 19, 2024)

I invite you to attempt Assignment 2 and to turn in your work for Questions 1–4. Any hand-written derivations should be submitted to me in hard copy. Any computational results should be collected in a single Wolfram Notebook and sent as an attachment to `kbeach@olemiss.edu`. Please follow the naming convention `Phys651-A2-webid.nb`, and be sure to include the subject line `Phys651-Fall2024-webid Assignment 2 Submission`.

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

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

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-valued elements. Recall that such Grassman numbers obey

$$\theta_i\theta_j = (\delta_{i,j} - 1)\theta_j\theta_i, \;\; \eta_i\eta_j = (\delta_{i,j} - 1)\eta_j\eta_i, \;\; \theta_i\eta_j = -\eta_j\theta_i$$

and that they support a unified integration/differential rule given by

$$\int d\theta\, \theta^\alpha = \frac{d}{d\theta}\theta^\alpha = \int d\eta\, \eta^\alpha = \frac{d}{d\eta}\eta^\alpha = \alpha \;\text{ for } (\alpha = 0, 1) \;\text{ and }\; \int d\eta\, \theta = \int d\theta\, \eta = 0.$$

   (a) For the $N = 2$ case, show explicitly that evaluation of the integral

$$\int d\eta_1\, d\eta_2\, d\theta_2\, d\theta_1\, \exp\left[\begin{pmatrix}\theta_1 & \theta_2\end{pmatrix}\begin{pmatrix}A_{1,1} & A_{1,2}\\ A_{2,1} & A_{2,2}\end{pmatrix}\begin{pmatrix}\eta_1\\ \eta_2\end{pmatrix}\right]$$

   yields $A_{1,1}A_{2,2} - A_{1,2}A_{2,1}$. Proceed by expanding $\exp(x) = 1 + x + x^2/2 + x^3/6 + \cdots$ in series.

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

   (c) Argue convincingly (in words, no explicit calculation is required) that the generic result is just $\det A$. The following *Mathematica* code may help to clarify your thinking.

```
buildA[n_] := Table[Subscript[A,i,j],{j,1,n},{i,1,n}]
buildA[2] // MatrixForm
buildA[3] // MatrixForm
Det[buildA[#]] & /@ Range[2, 4] // TableForm
ExplicitDet[M_, n_] := Total[Times @@@ Table[If[j == 1, Signature[#[[i]]], 1]
    Subscript[M, j, #[[i]][[j]]], {i, 1, n!}, {j, 1, n}] &[Permutations[Range[n]]]]
ExplicitDet[A, 2] == Det[buildA[2]]
ExplicitDet[A, 3] == Det[buildA[3]]
ExplicitDet[A, 4] == Det[buildA[4]]
And @@ Table[Expand[ExplicitDet[A, n]] == Expand[Det[buildA[n]]], {n, 2, 6}]
```

   (d) Since the Grassman variables obey an "exclusion principle" (viz., $\theta_i^2 = \eta_i^2 = 0$) and pick up a sign under "particle exchange" (viz., $\theta_1\theta_2 = -\theta_2\theta_1$), we can interpret the Grassman algebra as a description of fermionic degrees of freedom. The many-body wave function for a system of N (spinless) fermions is $\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = (N!)^{-1/2} \det A$, where $A_{i,j} = \psi_j(\mathbf{r}_i)$ 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 $\mathbf{r}_1$ and $\mathbf{r}_2$ take arbitrary values but $\psi_1 = \psi_2$; and (ii) if $\psi_1 \neq \psi_2$ but $\mathbf{r}_1 = \mathbf{r}_2$. Explain what your mathematical observations mean physically.

2. A ball tossed straight up into the air travels according to $h = v_0 t - \frac{1}{2} g t^2$. Here, v_0 is the initial ($t = 0$) vertical velocity, and g is the gravitational acceleration. 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	8.8
1.0	15.4
1.5	17.5
2.0	20.4
2.5	19.3
3.0	14.4
3.5	9.5

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

   (b) Construct the Moore-Penrose pseudoinverse by hand.

   (c) Give best estimates (in the least squares sense) of the initial velocity (v_0) and the gravitational acceleration (g). Check your answer against this *Mathematica* code.

```
tlist = {0.5, 1.0, 1.5, 2.0, 2.5, 3.0, 3.5}
hlist = {8.8, 15.4, 17.5, 20.4, 19.3, 14.4, 9.5};
x[t_] = v0 t - (g/2) t^2
xlist = 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] == Inverse[MT . M] . MT
PseudoInverse[M] . hlist
```

   (d) The observer has reported no "error bars" on the height measurements. Still, there are various ways (bootstrap methods especially) to estimate the uncertainty on the pseudoinverse values of v_0 and g, just based on the data given. One possibility is so-called jackknife resampling. Using that approach, one would compute the pseudoinverse solution 7 times on all possible 6-entry data sets produced by removing one row from the data table. This yields 7 estimates of v_0 and g, and the spread in those values can be interpreted as a fitting uncertainty. Write *Mathematica* code that carries out the jackknife procedure. You may want to make use of the `Mean` and `StandardDeviation` functions.

   (e) Make a plot that puts the jackknife fits through data points.

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 by hand. Confirm your results by comparing to *Mathematica*'s.

```
Table[{Subscript[\[Sigma], i], "=", MatrixForm[PauliMatrix[i]], " det =",
    Det[PauliMatrix[i]], " tr =", Tr[PauliMatrix[i]]}, {i, 1, 3}] // Grid
```

(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 2×2 identity matrix). Again, confirm your results:

```
MatrixForm /@ {PauliMatrix[1].PauliMatrix[1], MatrixPower[PauliMatrix[2], 2],
    MatrixPower[PauliMatrix[3], 2], -I PauliMatrix[1].PauliMatrix[2].PauliMatrix[3],
    IdentityMatrix[2]}
```

(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.

```
Table[MatrixForm /@ Table[PauliMatrix[a].PauliMatrix[b]
   + PauliMatrix[b].PauliMatrix[a], {b, 1, 3}], {a, 1, 3}] // TableForm
Table[MatrixForm[KroneckerDelta[a, b] 2 IdentityMatrix[2]], {b, 1, 3},
   {a, 1, 3}] // TableForm
```

(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; ϵ is the Levi-Civita symbol. Note that, in *Mathematica*, $\epsilon_{a,b,c} = 0, \pm 1$ coincides with `Signature[{a, b, c}]`:

```
Table[MatrixForm /@ Table[PauliMatrix[a].PauliMatrix[b] -
    PauliMatrix[b].PauliMatrix[a], {b, 1, 3}], {a, 1, 3}] // TableForm
Table[MatrixForm /@ Table[2 I Sum[Signature[{a, b, c}] PauliMatrix[c], {c, 1, 3}], {b,
    1, 3}], {a, 1, 3}] // TableForm
```

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

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

where $\theta = |\mathbf{n}|$ and $\hat{\mathbf{n}} = \mathbf{n}/\theta$ is a unit vector. The easiest approach is to apply the standard Taylor series expansions for the exponential, cosine, and sine functions.
You may want to remind yourself of these results:

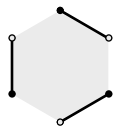
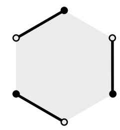
```
Sum[(-1)^k \[Theta]^k/k!, {k, 0, \[Infinity]}]
Sum[(-1)^k \[Theta]^(2 k)/((2 k)!), {k, 0, \[Infinity]}]
Sum[(-1)^k \[Theta]^(2 k + 1)/((2 k + 1)!), {k, 0, \[Infinity]}]
```

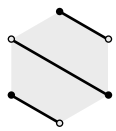
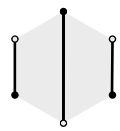
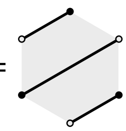
Here is a more elegantly typeset version of the last two lines of code.

```
c = HoldForm[Sum[(-1)^k \[Theta]^(2 k)/((2 k)!), {k, 0, \[Infinity]}]]
s = Sum[(-1)^k \[Theta]^(2 k + 1)/((2 k + 1)!), {k, 0, \[Infinity]}] // HoldForm
Row[{c, " \[LongEqual] ", ReleaseHold[c]}] // TraditionalForm
Row[{s, " \[LongEqual] ", ReleaseHold[s]}] // TraditionalForm
```

You may also want to make use of the fact that a unit vector dotted with itself is one ($\hat{\mathbf{n}}\cdot\hat{\mathbf{n}} = 1$, by definition) and that any vector crossed with itself vanishes ($\mathbf{u}\times\mathbf{u} = 0$).

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 overlap 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}). I encourage you to make your life easier by seeking computer assistance. You are welcome to determine the loop counts by hand—since that part of the computation is trickiest—but everything else can be easily automated.

The elements $L_{i,j}$ correspond to `L[[i,j]]` in *Mathematica*. You should find that the nested array of elements looks like

```
L = {{3, 1, 2, 2, 2}, {1, 3, 2, 2, 2}, ..., {2, 2, 1, 1, 3}}
```

(b) This basis is not orthonormal. Show that the resolution of unity is $\hat{\mathbb{1}} = \sum_{i=1}^{5}\sum_{j=1}^{5}|i\rangle S^{-1}_{i,j}\langle j|$. 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 (each black connecting to a white) 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 sometimes loosely referred to as the square root of the matrix S but is more properly understood as a positive-definite decomposition or Cholesky decompostition. Such a decomposition is not unique.

(e) Take as a starting point two states

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

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 the collection of kets $\{|u_1\rangle, |u_2\rangle, |u_3\rangle\}$ constitutes 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!