Physics 241– Quantum Magnetism

Problem Set 4 **Due 2/10/03**

[**1.**] Figure out the path integral representation for the partition function $Z = \mathrm{Tr}[e^{-\beta H}]$ of a spin-1/2 particle with Hamiltonian $H = -hS_z - tS_x$. (You can set $\hbar = 1$ for convenience.) To do this, follow the procedure in class: Discretize β into L intervals of length τ. Then approximate $e^{-\tau H} \approx e^{-\tau h S_z} e^{-\tau S_x}$. Insert complete sets of states (e.g. in the S_z basis). Hint: Can you figure out a value for the real constant a which satisfies $e^{a S_z^l S_z^{l+1}} = \langle S_z^l | e^{t\tau S_x} | S_z^{l+1} \rangle$ for all four matrix elements?

[**2.**] Compute the exact partition function of the Hamiltonian in problem 1. (Do it two ways, first, by diagonalizing an appropriate 2x2 matrix, then by thinking of H as $H = -B \cdot S$ and rotating your coordinate axes so that B is in the z direction.) Then compute $\langle S_z \rangle$.

[**3.**] Write a program which evaluates

$$\begin{aligned}
\tfrac{1}{2} m\omega^2 \langle x^2 \rangle &= \frac{1}{4L} m\omega^2 \sum_l \frac{1}{\lambda_l}, \\
\lambda_l &= \tfrac{1}{2} m\omega^2 \tau + \frac{m}{\tau}[1 - \cos(k_l)], \\
k_l &= 2\pi l / L \\
l &= 1, 2, \ldots L.
\end{aligned}$$

Choose the value $m = 3$ and $\omega = \frac{1}{2}$ and plot the result for the sum versus τ (keeping the product $L\tau = \beta$ fixed.) Show the result comes in to

$$P = \tfrac{1}{2}\omega\left(\frac{1}{e^{\beta\omega} - 1} + \tfrac{1}{2}\right),$$

as $\tau \to 0$.

[**4.**] *Optional:* Choose *either* the quantum oscillator *or* the Hamiltonian considered in problems 1 and 2. Write a Monte Carlo program to solve for $\langle S_z \rangle$ (problems 1, 2) or $\langle \frac{1}{2} m\omega^2 x^2 \rangle$ (quantum oscillator). Show you get the right answer. How long do you need to run your program? Are you able to get the statistical error bars small enough that you can see the error associated with finite τ?