Phys 472 Assignment 8 Due Nov. 6, 2020, before 9:00 am Marsiglio, Fall 2020

For Question 2 especially, be certain to include your programs!!!

1. Consider the Dirac equation for a free particle, and assume the solution consists of plane wave states with definite momentum p. Find the eigenvalues (there ought to be 4 of them!). They are both doubly degenerate. Explain why. Also explain how Dirac interpreted the two non-degenerate solutions (you may have to look up references for this explanation — include these in your explanation).

2. The problem of a particle of mass m_0 in a well of the form $V(x) = \lambda x^4$ cannot easily be solved. Hence, we revert to a variational calculation. If nothing else, this will tell us about the units in the problem, which could also be determined through dimensional analysis.

(a) Use a Gaussian trial wave function,

$$\psi(x) = A_\alpha e^{-\alpha x^2/2}.$$

First determine A_α, and then use the variational principle to determine E_{gs} where gs stands for "ground state." *Answer:* $E_{gs} = (\frac{3}{4})(3^{1/3})\left(\frac{\hbar^2}{2m_0}\right)^{2/3}\lambda^{1/3} \approx 1.08\left(\frac{\hbar^2}{2m_0}\right)^{2/3}\lambda^{1/3}$.

(b) As you can see, the answer gives us the units in which the energy is most readily expressed. But we have no idea how accurate this is — all we know is that the true energy is somewhat lower. Well, not really — we are in fact well-equipped to work out the exact answer. Place the potential in an infinite square well between $0 \le x \le a$ — therefore it should have the form $V(x) = \lambda(x - a/2)^4$. Use the usual basis set, $\phi_j(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{j\pi x}{a}\right)$, and, using $\psi(x) = \sum c_j\phi_j(x)$, construct the matrix elements for the eigenvalue equation,

$$\sum_{j=1}^{N_{\max}} H_{ij}c_j = Ec_i,$$

where $H_{ij} = K_{ij} + V_{ij}$, and K_{ij} is the usual kinetic energy,

$$K_{ij} = j^2 E_1^{(0)}\delta_{ij},$$

and

$$V_{ij} = \lambda\frac{2}{a}\int_0^a dx \sin\left(\frac{i\pi x}{a}\right)\left(x - \frac{a}{2}\right)^4 \sin\left(\frac{j\pi x}{a}\right).$$

Here $E_1^{(0)} \equiv \hbar^2\pi^2/(2m_0a^2)$. Derive that

$$V_{ij} = \lambda a^4\left[J_4(i-j) - J_4(i+j)\right] \equiv \lambda a^4 F_{ij},$$

where

$$J_4(n) = \delta_{n,0}\frac{1}{80} + (1-\delta_{n,0})\frac{1+(-1)^n}{2}\left(\frac{1}{(n\pi)^2} - \frac{24}{(n\pi)^4}\right).$$

and so F_{ij} are just numbers. We require a common energy scale, and so we use $E_1^{(0)}$. Therefore

$$\frac{H_{ij}}{E_1^{(0)}} = j^2\delta_{ij} + \lambda a^4 \frac{2m_0}{\hbar^2}\frac{a^2}{\pi^2}F_{ij} \equiv \pi^4 s^6 F_{ij},$$

where we have defined the dimensionless parameter s through the second equality. Solve this problem numerically, by exact diagonalization. To compare with previous results, once you obtain this numerical (dimensionless) energy, express it in terms of energy units as in part (a), i.e. $\left(\frac{\hbar^2}{2m_0}\right)^{2/3}\lambda^{1/3}$. If ϵ_n is the dimensionless energy (in units of $E_1^{(0)}$ obtained in your program, then derive that the energy is given by

$$E_n = \left(\frac{\hbar^2}{2m_0}\right)^{2/3}\lambda^{1/3}\frac{\epsilon_n}{s^2}. \qquad (A)$$

To get actual values of ϵ you will need a value of s. Normally you would need to experiment with this, so try $s = 1$, $s = 2$, $s = 5$, and $s = 10$. You should notice convergence of the ground state energy, and for the last three values of s in particular, the answer will be the same, independent of s. Present a table of these ground state energy values, as expressed in Eq. (A) above, for the 3 values of s. *Converged answer: 1.060362 (I used $N_{\max} = 800$, but you should get this will much smaller values of $N_{\max}$. Note how close your answer in (a) is to the exact answer.*

(c) Present a plot of the exact energy (in units of $\left(\frac{\hbar^2}{2m_0}\right)^{2/3}\lambda^{1/3}$) vs. eigenvalue index n, for the 4 values of s referred to in (b). Use a scale of $n = 1$ to 400, and E (in units of $\left(\frac{\hbar^2}{2m_0}\right)^{2/3}\lambda^{1/3}$) from 0 to 8000. Indicate which results are indicative of the λx^4 potential (i.e. no longer depend on s, which represents a choice of a.)

(d) You will have noticed that for large values of n, the results in (c) become unreliable. For example, we can focus on $s = 5$; the results in (c) indicate that beyond a certain value of n the energy is no longer that of the pure quartic potential under study, but also reflect the confinement of the infinite square well (like the upturn in energies visible in Fig. 1 of the 2009 reference that you reproduced in Assignment 2). Having now studied perturbation theory, we can now understand this upturn in the energy at large values of n by treating the quartic potential as a perturbation. Given an infinite square well with width a (and as represented by the parameter s in the current context) as the main system, treat the quartic potential as a perturbation. Calculate the correction to the eigenvalues using first order perturbation theory (with $\hat{H}_0$ given by the infinite square well. Write this in units of $\left(\frac{\hbar^2}{2m_0}\right)^{2/3}\lambda^{1/3}$, and keep terms for large n values only. For $s = 5$ only, plot the exact results again, along with $E_n^{(0)} = n^2/s^2$, and $E_n^{(0)} + E_n^{(1)}$ vs n. Use axis ranges $0 < n < 400$ and $0 < E < 8000$ (again with units of $\left(\frac{\hbar^2}{2m_0}\right)^{2/3}\lambda^{1/3}$. Note how this expression comes very close to agreeing with the exact results for large values of n.

Partial answer: $E_n^{(1)} + E_n^{(1)} = \left(\frac{\hbar^2}{2m_0}\right)^{2/3}\lambda^{1/3}\left(n^2/s^2 + \pi^4 s^4/80\right)$.

(e) Now we will come full circle and relate the exact matrix approach to the variational method. Once again, we tackle the problem of a quartic potential, but we seek a suitable basis that does not require an infinite square well that (irritatingly) truncates the potential of interest (and also (irritatingly) requires a shift away from the origin of $a/2$). Such a basis exists in the eigenstates of the harmonic oscillator potential. In fact in part (a) we used the ground state for the harmonic oscillator potential as a variational wave function. Not only did we do that, but we used the variational principle to determine for us *which* harmonic oscillator potential we should use — there are an infinite number of them, characterized in (a) by the parameter $\alpha \equiv m_0\omega/\hbar$, where ω is the characteristic frequency of the harmonic oscillator potential. In (a) we found which value of $m_0\omega/\hbar$ we should use. Derive the value of $\hbar\omega$ to which this corresponds. *Answer:* $\hbar\omega = 2(3^{1/3})\left(\frac{\hbar^2}{2m_0}\right)^{2/3}\lambda^{1/3}$.
Now adopt this basis set (use the kets $|n\rangle$ to avoid doing any integrals!), and derive the matrix elements for the Hamiltonian

$$\hat{H} = \frac{p^2}{2m_0} + \lambda x^4$$

written in this harmonic oscillator basis. [That is, having expanded the wave function ψ as

$$\psi\rangle = \sum_{n=0}^{N_{max2}} c_n|n\rangle,$$

then we arrive at the usual matrix equation, except now the coefficients are for the harmonic oscillator basis set,

$$\sum_{j=0}^{N_{max2}} H_{ij}c_j = Ec_i$$

where

$$H_{ij} \equiv \langle i|\hat{H}|j\rangle].$$

Determine expressions for H_{ij}. *Partial answer:*
$\frac{1}{2m_0}\langle i|p^2|j\rangle = -\frac{\hbar\omega}{4}\left[\sqrt{(j+2)(j+1)}\delta_{i,j+2} + \sqrt{j(j-1)}\delta_{i,j-2} - (2j+1)\delta_{i,j}\right]$.
The elements $\langle i|x^4|j\rangle$ *have terms proportional to* δ_{ij}, $\delta_{i,j\pm2}$, *and* $\delta_{i,j\pm4}$.
Finally, diagonalize this Hamitonian and (hopefully) get the same result as in (b). Show the result for the ground state energy as a function of $N_{\rm max2}$ (say for $N_{\rm max2} = 1, 2, 5, 10, 50$). Note that for $N_{\rm max2} < \infty$ (and same for $N_{\rm max}$ too!) the exact matrix diagonalization method is entirely a variational calculation (known as a "controlled" variational calculation)!