Università degli Studi di Trento – Dipartimento di Fisica

Computational Physics 1

Recitation class, April 14, 2021

Quantum bound states

Indice

1 A one dimensional potential

Use the Numerov algorithm and direct diagonalization to evaluate the energies of *all* the bound states of a quantum particle of mass m moving in a one-dimensional potential

$$v(x) = \frac{v_0}{\cosh^4\left(\frac{x}{a}\right)}, \tag{1}$$

with $v_0 < 0$. Denoting

$$\xi = \frac{\hbar^2}{ma^2|v_0|}.$$

consider the cases $\xi \in [0.05, 0.01, 0.005]$.

2 The neon dimer

Calculate the energies of *all* the bound states of the ^{20}Ne dimer, assuming a Lennard-Jones potential with $\varepsilon/k_\mathrm{B} = 35.7$ K and $\sigma = 2.79$ Å.

3 C wrappers

Please be inspired by the provided examples.

3.1 Hermitean dense matrices

Before solving the next problems, try to write your C wrapper to the LAPACK routines performing diagonalization of hermitean double-precision complex matrices. Double-precision complex (z), hermitean (he), eigenvalues (ev). In LAPACK speak this is, of course, `zheev`.

3.2 Only a few eigenvectors

Some routines provide only a subset of the eigenvectors, for example LAPACK's `dsyevr`. Write wrappers to find only the first $m \leq n$ eigenvectors of a $n \times n$ symmetric or hermitean matrices.

4 A periodic square well

Calculate the dispersion relation $E_n(K)$ of a quantum particle of mass m in a *periodic* potential that, in a unit cell of size a is given by

$$v(x) = \begin{cases} -v_0 & 0 \leq x \leq b \\ 0 & x > b \end{cases} \tag{2}$$

for $b/a = 0.3$, considering the case in which

$$\frac{\hbar^2}{2ma^2 v_0} = 1,$$

and for $n = 0, 1, 2$. Compare the results with the analytic solution that you can find in Wikipedia.

5 A periodic gaussian well

Calculate the dispersion relation $E_n(K)$ of a quantum particle of mass m in a *periodic* potential that, in a unit cell of size a is given by

$$v(x) = -v_0 \exp\left[-\frac{(x - a/2)^2}{2b^2}\right] \tag{3}$$

for $b/a = 0.3$, $v_0 > 0$,

$$\frac{\hbar^2}{2ma^2 v_0} = 1,$$

and $n = 0, 1, 2$.