

# SAIP2014



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## **Norm conserving pseudopotentials for 1-D systems**

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### **Abstract :**

We have devised norm-conserving pseudopotentials for several non-interacting 1-D quantum mechanical systems namely, the infinite square well, finite square well, simple harmonic oscillator and hydrogen atom. The purpose of this study is to develop simple computational exercises to teach undergraduate and graduate students particular theoretical and numerical aspects of the pseudopotential method which is an essential aspect of modern electronic structure software, and which many graduate students do not understand, in spite of them using these codes for their research. We compare logarithmic derivatives, as well as energies of appropriate excited states of the real and pseudo systems to determine the transferability of the calculated pseudopotentials. We obtain highly transferable pseudopotentials for the hydrogen atom, moderately transferable pseudopotentials for the infinite square well and poorly transferable pseudopotentials for the finite square well and simple harmonic oscillator.

### **Award :**

No

### **Level :**

N/A

### **Supervisor :**

n/a

### **Paper :**

No

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