Variational Monte Carlo studies of quantum mechanical systems (WIP title)

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Abstract

1 Introduction

2 Some Pandoc Markdown syntax

I'm sure you're both familiar with the common Markdown syntax, and this applies just as well here. Pandoc exports links to the compiled PDF, so I often use them liberally, like this. If you want *inline math*, you just write a set of dollar signs, like this: $f(x) = \sin(x)$. Most commonly though, you'll probably want *display math*, which is just as simple to write. Be sure to have a couple of newlines as padding, and just use a double set of dollar signs, like this:

$$E(\alpha) = \frac{\langle\psi(\alpha)|\mathcal{H}|\psi(\alpha)\rangle}{\langle\psi(\alpha)|\psi(\alpha)\rangle}$$

By default, these are not numerated (which I think is sensible). However, if you want them numerated, you just use the following syntax to assign a label

$$E_L(X) = \frac{\mathcal{H}\psi(X,\alpha)}{\psi(X,\alpha)}, \tag{1}$$

and then reference the equation by using the same label. See eq. (1) (beware that this will not show up in the Markdown Preview pane. You'll need to compile the document to see the result).

One thing I find quite useful is to use footnotes throughout the document to give short insights (especially in the theory part). This is simple with Pandoc;

just use this syntax[1]. In addition, we can site all references (defined in the `kodb.yaml`-file) with this syntax (see Aasrud, Rongve, and Raniseth 2019).

3 Theory

3.1 The system described

The system in question is a hard sphere Bose gas. The system is affected by an external potential - an *elliptical harmonic trap* - that is described by the following equation:

$$V_{\text{ext}}(\mathbf{r}) = \frac{1}{2}m\left(\omega_{\text{ho}}^2(x^2+y^2)+\omega_z z^2\right). \tag{2}$$

Note that setting $\omega_{\text{ho}} = \omega_z$ results in eq. (2) evaluating to $V_{\text{ext}} = \frac{1}{2}m\omega_{\text{ho}}^2 r^2$, which represents the *spherical* case of the elliptical harmonic trap. In addition to this external potential, we represent the inter-boson interactions with the following pairwise, repulsive potential:

$$V_{\text{int}}(|\mathbf{r}_i - \mathbf{r}_j|) = \begin{cases} \infty & |\mathbf{r}_i - \mathbf{r}_j| \leq a \\ 0 & |\mathbf{r}_i - \mathbf{r}_j| > a \end{cases}. \tag{3}$$

Eq. (2) and eq. (3) evaluate to the following two-body Hamiltonian:

$$H = \sum_i^N \left(-\frac{\hbar^2}{2m}\nabla_i^2 + V_{\text{ext}}(\mathbf{r}_i)\right) + \sum_{i<j}^N V_{\text{int}}(|\mathbf{r}_i - \mathbf{r}_j|).$$

The index notation used here is described in A.2.1.

3.2 Wave function of the system

For a system of N particles, we use the following trial wave function:

$$\Psi_T(\mathbf{r}_1, ..., \mathbf{r}_N, \alpha, \beta) = \prod_i g(\alpha, \beta, \mathbf{r}_i) \prod_{j<k} f(a, |\mathbf{r}_j - \mathbf{r}_k|). \tag{4}$$

Once again, note the index notation explained in A.2.1.

[1] Welcome to the footer! How are you?

A Appendix

A.1 Source code

All source code for both the Rust VMC implementation and this document is found on the following GitHub Repository

https://github.com/kmaasrud/vmc-fys4411

A.2 Notation and other explanations

A.2.1 Index notation for sums and products

For products and sums, the following convention is used:

$$\sum_{i<j}^{N} = \sum_{i=1}^{N} \sum_{j=i+1}^{N}, \quad \text{or} \quad \prod_{i<j}^{N} = \prod_{i=1}^{N} \prod_{j=i+1}^{N}$$

A.3 Derivations

References

Aasrud, K. M., A. S. Rongve, and A. M. Raniseth. 2019. "Project 3." https://github.com/kmaasrud/gq-mcm-fys3150/blob/master/doc/Project-3_Aasrud-Raniseth-Rongve.pdf.