VMC

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Abstract

Author's comments: .

1 Introduction

In order to write this project paper and the code required to produce the results, I used a variety of tools, including: Python 3.7.5, NumPy [1], , as well as a number of books, web-pages and articles - of which most are listed under references. All the code required to reproduce the results may be found on my github page .

2 Material and methods

2.1 System

Hard sphere Bose gas for various number of particles. In order to study the properties of the system, a trial wave function (5) is used. Trap is an harmonic spherical (S) ($\omega_{ho}^2 = \omega_z^2$) or elliptical (E) ($\omega_{ho}^2 \neq \omega_z^2$) one, two and finally three dimensional trap, made up of the potential (1). The two-body Hamiltonian of the system

$$V_{ext}(\mathbf{r}) = \begin{cases} \frac{1}{2}m\omega_{ho}^2 r^2 & (S) \\ \frac{1}{2}m[\omega_{ho}^2(x^2+y^2) + \omega_z^2 z^2] & (E) \end{cases} \tag{1}$$

Where ω_{ho}^2 is the trap potential strength.

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

as the two-body Hamiltonian of the system. Here ω_{ho}^2 defines the trap potential strength. In the case of the elliptical trap, $V_{ext}(x, y, z)$, $\omega_{ho} = \omega_\perp$ is the trap frequency in the perpendicular or xy plane and ω_z the frequency in the z direction. The mean square vibrational amplitude of a single boson at $T = 0K$ in the trap (1) is $\langle x^2 \rangle = (\hbar/2m\omega_{ho})$ so that $a_{ho} \equiv (\hbar/m\omega_{ho})^{\frac{1}{2}}$ defines the characteristic length of the trap. The ratio of the frequencies is denoted $\lambda = \omega_z/\omega_\perp$ leading to a ratio of the trap lengths $(a_\perp/a_z) = (\omega_z/\omega_\perp)^{\frac{1}{2}} = \sqrt{\lambda}$. Note that we use the shorthand notation

$$\sum_{i<j}^N V_{ij} \equiv \sum_{i=1}^N \sum_{j=i+1}^N V_{ij}, \tag{3}$$

that is, the notation $i < j$ under the summation sign signifies a double sum running over all pairwise interactions once.

$$V_{int}(|\mathbf{r}_i - \mathbf{r}_j|) = \begin{cases} \infty & |\mathbf{r}_i - \mathbf{r}_j| \leq a \\ 0 & |\mathbf{r}_i - \mathbf{r}_j| > a \end{cases} \tag{4}$$

$$\Psi_T(\mathbf{r}) = \Psi_T(\mathbf{r}_1, \mathbf{r}_2, \dots \mathbf{r}_N, \alpha, \beta) = \left[\prod_i g(\alpha, \beta, \mathbf{r}_i) \right] \left[\prod_{j<k} f(a, |\mathbf{r}_j - \mathbf{r}_k|) \right], \tag{5}$$

Where

$$g(\alpha, \beta, \mathbf{r}_i) = \exp\left[-\alpha(x_i^2 + y_i^2 + \beta z_i^2)\right]. \tag{6}$$

For spherical traps we have $\beta = 1$ and for non-interacting bosons ($a = 0$) we have $\alpha = 1/2a_{ho}^2$. The correlation wave function is

$$f(a, |\mathbf{r}_i - \mathbf{r}_j|) = \begin{cases} 0 & |\mathbf{r}_i - \mathbf{r}_j| \leq a \\ (1 - \frac{a}{|\mathbf{r}_i - \mathbf{r}_j|}) & |\mathbf{r}_i - \mathbf{r}_j| > a. \end{cases} \tag{7}$$

2.2 Local energy

The local energy is defined as (12). Using the trial wave function (5), the first thingything is to find the analytical expression IOT save flops (quote with ratio).

$$E_L(\mathbf{r}) = \frac{1}{\Psi_T(\mathbf{r})} H\Psi_T(\mathbf{r}), \tag{8}$$

2.2.1 Non-interacting

In the Non-interacting case, the local energy (12) on the trial wave functio eqrefeq:trialwf with $a = 0$ -> only HO potential and $\beta = 1$. This also means that the internal potential V_{int} in the Hamiltonian (2) becomes zero.

$$E_L(\mathbf{r})\Psi_T(\mathbf{r}) = \frac{1}{\prod_i g(\alpha, \beta, \mathbf{r}_i)} \sum_i^N \left(\frac{-\hbar^2}{2m} \nabla_i^2 + V_{ext}(\mathbf{r}_i) \right) \left[\prod_i g(\alpha, \beta, \mathbf{r}_i) \right] \tag{9}$$

Taking the gradient of g:

$$\nabla_i g(\alpha, \beta, \mathbf{r}_i) = -2\alpha \mathbf{r}_i g(\alpha, \beta, \mathbf{r}_i) \tag{10}$$

Taking the Laplacian of the g thing which I'm sure has another name. From the product rule, this entails deriving $\mathbf{r}_i$, resulting in a coefficient d representing the dimensionality of r.

$$\nabla_i^2 g(\alpha, \beta, \mathbf{r}_i) = (-2d\alpha + 4\alpha \mathbf{r}_i^2) g(\alpha, \beta, \mathbf{r}_i) \tag{11}$$

Meaning that

$$E_L(\mathbf{r}) = \sum_i^N \left(\frac{-\hbar^2}{2m} (-2d\alpha + 4\alpha \mathbf{r}_i^2) + \frac{1}{2} m\omega_{ho}^2 r_i^2 \right) \tag{12}$$

Using natural units, $\hbar = c = 1$, and unity mass $m = 1$, the equation becomes;

$$E_L(\mathbf{r}) = \alpha d N + \left(-2\alpha + \frac{1}{2}\omega_{ho}^2 \right) \sum_i^N r_i^2 \tag{13}$$

(11) also leads to an analytic expression for the drift force used in the importance sampling;

$$F_i = \frac{2\nabla\Psi_T}{\Psi_T} = -4\alpha \mathbf{r}_i \tag{14}$$

2.2.2 Interacting - IKKE FERDIG

Next, we will find the local energy for the full problem in three dimensions. The tricky part is to find an analytic expressions for the derivative of the trial wave function

$$\frac{1}{\Psi_T(\mathbf{r})} \sum_i^N \nabla_i^2 \Psi_T(\mathbf{r}),$$

with the above trial wave function of Eq. (5). We rewrite

$$\Psi_T(\mathbf{r}) = \Psi_T(\mathbf{r}_1, \mathbf{r}_2, \dots \mathbf{r}_N, \alpha, \beta) = \left[\prod_i g(\alpha, \beta, \mathbf{r}_i)\right] \left[\prod_{j<k} f(a, |\mathbf{r}_j - \mathbf{r}_k|)\right],$$

as

$$\Psi_T(\mathbf{r}) = \left[\prod_i g(\alpha, \beta, \mathbf{r}_i)\right] \exp\left(\sum_{j<k} u_{jk}\right)$$

where we have defined $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ and

$$\prod_{i<j} f(r_{ij}) = \exp\left(\sum_{i<j} u_{jk}\right),$$

with $u_{jk} = \ln f(r_{ij})$. We have also

$$g(\alpha, \beta, \mathbf{r}_i) = \exp\left[-\alpha(x_i^2 + y_i^2 + \beta z_i^2)\right] = \phi(\mathbf{r}_i) = \phi_i.$$

Taking the gradient with respect to the k'th particle;

$$\nabla_k \Psi_T(\mathbf{r}) = \nabla_k \left(\left[\prod_i \phi_i\right] \exp\left(\sum_{j<m} u_{jm}\right)\right) \tag{15}$$

$$= \left(\nabla_k \left[\prod_i \phi_i\right]\right) \exp\left(\sum_{j<m} u_{jm}\right) + \left[\prod_i \phi_i\right] \left(\nabla_k \exp\left(\sum_{j<m} u_{jm}\right)\right) \tag{16}$$

The gradient of the non-interacting part of the TW:

$$\nabla_k \left[\prod_i \phi_i\right] = \nabla_k \phi_k \left[\prod_{i \neq k} \phi_i\right] = \nabla_k \phi_k \frac{\prod_i g(\alpha, \beta, \mathbf{r}_i)}{\phi_k} \tag{17}$$

$$\tag{18}$$

And the gradient of the interacting part, remembering that $r_{kl} = r_{lk}$;

$$\nabla_k \exp\left(\sum_{j<m} u_{jm}\right) = \exp\left(\sum_{j<m} u_{jm}\right) \sum_{j \neq k} \nabla_k u_{kj} = \prod_{j<m} f(r_{jm}) \sum_{l \neq k} \nabla_k u_{kl} \tag{19}$$

Thus (16) is

$$\begin{aligned} \nabla_k \Psi_T(\mathbf{r}) = \nabla_k \phi_k \left[\prod_{i \neq k} \phi_i\right] \exp\left(\sum_{j<m} u_{jm}\right) \\ + \left[\prod_i \phi_i\right] \exp\left(\sum_{j<m} u_{jm}\right) \sum_{l \neq k} \nabla_k u_{kl} \end{aligned} \tag{20}$$

or

$$
\begin{aligned}
\nabla_k \Psi_T(\mathbf{r}) &= \nabla_k \phi_k \frac{\prod_i g(\alpha,\beta,\mathbf{r}_i)}{\phi_k} \prod_{j<m} f(r_{jm}) \\
&\quad + \prod_i g(\alpha,\beta,\mathbf{r}_i) \prod_{j<m} f(r_{jm}) \sum_{l\neq k} \nabla_k u_{kl} \\
&= \left(\frac{\nabla_k \phi_k}{\phi_k} + \sum_{l\neq k} \nabla_k u_{kl} \right) \Psi_T(\mathbf{r})
\end{aligned}
\tag{21}
$$

Next, we find the second derivative;

$$
\begin{aligned}
\frac{1}{\Psi_T(\mathbf{r})} \nabla_k^2 \Psi_T(\mathbf{r}) &= \frac{1}{\Psi_T(\mathbf{r})} \nabla_k \left(\left(\frac{\nabla_k \phi_k}{\phi_k} + \sum_{l\neq k} \nabla_k u_{kl} \right) \Psi_T(\mathbf{r}) \right) \\
&= \frac{1}{\Psi_T(\mathbf{r})} \left(\left(\phi_k \nabla_k \frac{1}{\phi_k} + \frac{\nabla_k^2 \phi_k}{\phi_k} + \sum_{l\neq k} \nabla_k^2 u_{kl} \right) \Psi_T(\mathbf{r}) + \left(\frac{\nabla_k \phi_k}{\phi_k} + \sum_{l\neq k} \nabla_k u_{kl} \right)^2 \Psi_T(\mathbf{r}) \right) \\
&= \left(\frac{\nabla_k \phi_k}{\phi_k} \right)^2 + \frac{\nabla_k^2 \phi_k}{\phi_k} + \sum_{l\neq k} \nabla_k^2 u_{kl} + \left(\frac{\nabla_k \phi_k}{\phi_k} + \sum_{l\neq k} \nabla_k u_{kl} \right)^2 \\
&= -\left(\frac{\nabla_k \phi_k}{\phi_k} \right)^2 + \frac{\nabla_k^2 \phi_k}{\phi_k} + \sum_{l\neq k} \nabla_k^2 u_{kl} + \left(\frac{\nabla_k \phi_k}{\phi_k} \right)^2 + 2 \left(\frac{\nabla_k \phi_k}{\phi_k} \sum_{l\neq k} \nabla_k u_{kl} \right) + \left(\sum_{l\neq k} \nabla_k u_{kl} \right)^2 \\
&= \frac{\nabla_k^2 \phi_k}{\phi_k} + 2 \frac{\nabla_k \phi_k}{\phi_k} \sum_{l\neq k} \nabla_k u_{kl} + \sum_{l\neq k} \nabla_k^2 u_{kl} + \left(\sum_{l\neq k} \nabla_k u_{kl} \right)^2
\end{aligned}
\tag{22}
$$

In order to simplify applying the ∇_k-operator to u_{kl}, the operator is re-written:

$$
\nabla_k = \nabla_k \frac{\partial r_{kl}}{\partial r_{kl}} = \nabla_k \sqrt{(\boldsymbol{r}_k - \boldsymbol{r}_l)^2} \frac{\partial}{\partial r_{kl}} = \frac{\boldsymbol{r}_k - \boldsymbol{r}_l}{r_{kl}} \frac{\partial}{\partial r_{kl}}
$$

This re-written operator is then applied to the $\nabla_k u_{kl}$ terms, such that

$$
\nabla_k u_{kl} = \frac{\boldsymbol{r}_k - \boldsymbol{r}_l}{r_{kl}} \frac{\partial u_{kl}}{\partial r_{kl}} = \frac{\boldsymbol{r}_k - \boldsymbol{r}_l}{r_{kl}} u'_{kl}
$$

And

$$
\begin{aligned}
\nabla_k^2 u_{kl} &= \left(\nabla_k \frac{\boldsymbol{r}_k - \boldsymbol{r}_l}{r_{kl}}\right) \partial u'_{kl} + \frac{\boldsymbol{r}_k - \boldsymbol{r}_l}{r_{kl}} \left(\nabla_k u'_{kl}\right) \\
&= \left(\frac{\nabla_k (\boldsymbol{r}_k - \boldsymbol{r}_l)}{r_{kl}}\right) u'_{kl} + (\boldsymbol{r}_k - \boldsymbol{r}_l) \left(\nabla_k \frac{1}{r_{kl}}\right) u'_{kl} + \frac{\boldsymbol{r}_k - \boldsymbol{r}_l}{r_{kl}} \left(\nabla_k u'_{kl}\right) \\
&= \frac{d}{r_{kl}} u'_{kl} - (\boldsymbol{r}_k - \boldsymbol{r}_l) \frac{(\boldsymbol{r}_k - \boldsymbol{r}_l)}{r_{kl}^3} u'_{kl} + \left(\frac{\boldsymbol{r}_k - \boldsymbol{r}_l}{r_{kl}}\right)^2 u''_{kl} \\
&= \left(\frac{d}{r_{kl}} - \frac{(\boldsymbol{r}_k - \boldsymbol{r}_l)^2}{r_{kl}^3}\right) u'_{kl} + \left(\frac{\boldsymbol{r}_k - \boldsymbol{r}_l}{r_{kl}}\right)^2 u''_{kl}
\end{aligned}
$$

Where $(\boldsymbol{r}_k - \boldsymbol{r}_l)^2 = {r_{kl}}^2$, thus

$$
\nabla_k^2 u_{kl} = \left(\frac{d}{r_{kl}} - \frac{1}{r_{kl}}\right) u'_{kl} + u''_{kl} = \frac{d-1}{r_{kl}} u'_{kl} + u''_{kl}
$$

Applied to the Laplacian;

$$
\begin{aligned}
\frac{1}{\Psi_T(\mathbf{r})} \nabla_k^2 \Psi_T(\mathbf{r}) = \frac{\nabla_k^2 \phi_k}{\phi_k} &+ 2 \frac{\nabla_k \phi_k}{\phi_k} \sum_{l \neq k} \frac{\boldsymbol{r}_k - \boldsymbol{r}_l}{r_{kl}} u'_{kl} \\
&+ \left(\sum_{l \neq k} \frac{\boldsymbol{r}_k - \boldsymbol{r}_l}{r_{kl}} \partial u'_{kl} \right)^2 \\
&+ \sum_{l \neq k} \left(\frac{d-1}{r_{kl}} u'_{kl} + u''_{kl} \right)
\end{aligned} \tag{23}
$$

Expanding the third term, re-arranging, and inserting $d = 3$;

$$
\begin{aligned}
\frac{1}{\Psi_T(\mathbf{r})} \nabla_k^2 \Psi_T(\mathbf{r}) = \frac{\nabla_k^2 \phi_k}{\phi_k} &+ 2 \frac{\nabla_k \phi_k}{\phi_k} \sum_{l \neq k} \frac{\boldsymbol{r}_k - \boldsymbol{r}_l}{r_{kl}} u'_{kl} \\
&+ \sum_{j \neq k} \sum_{l \neq k} \frac{(\boldsymbol{r}_k - \boldsymbol{r}_l)(\boldsymbol{r}_k - \boldsymbol{r}_j)}{r_{kj} r_{kl}} u'_{kj} u'_{kl} \\
&+ \sum_{l \neq k} \left(u''_{kl} + \frac{2}{r_{kl}} u'_{kl} \right)
\end{aligned} \tag{24}
$$

3 Results

4 Conclusions

References

[1] Travis E Oliphant. *A guide to NumPy*, volume 1. Trelgol Publishing USA, 2006.

Appendices

Appendix 1.