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

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

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 care, 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

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

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

$$F_i = \frac{2\nabla \Psi_T}{\Psi_T} = -4\alpha \mathbf{r}_i \tag{13}$$

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 (and we can use the same general expressions for projects 2 and 3)

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

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;

$$\nabla_k \Psi_T(\mathbf{r}) = \nabla_k \left(\left[\prod_i \phi_i\right] \exp\left(\sum_{j<m} u_{jm}\right)\right) \tag{14}$$

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

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

$$\nabla_k \left[\prod_i \phi_i\right] = \nabla_k \phi_k \left[\prod_{i\neq k} \phi_i\right] = \nabla_k \phi_k \frac{\prod_i g(\alpha,\beta,\mathbf{r}_i)}{\phi_k} \tag{16}$$

$$\tag{17}$$

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

$$\nabla_k \exp\left(\sum_{j<m} u_{jm}\right) = \exp\left(\sum_{j<m} u_{jm}\right) \sum_{j\neq k} \nabla_k u_{kj} = \prod_{j<m} f(r_{jm}) \sum_{l\neq k} \nabla_k u_{kl} \tag{18}$$

Thus (15) is

$$\begin{aligned} \nabla_k \Psi_T(\mathbf{r}) = \nabla_k \phi_k \left[\prod_{i\neq k} \phi_i\right] \exp\left(\sum_{j<m} u_{jm}\right) \\ + \left[\prod_i \phi_i\right] \exp\left(\sum_{j<m} u_{jm}\right) \sum_{l\neq k} \nabla_k u_{kl} \end{aligned} \tag{19}$$

or

$$
\begin{aligned}
\nabla_k \Psi_T(\mathbf{r}) &= \nabla_k \phi_k \frac{\prod_i g(\alpha,\beta,\mathbf{r}_i)}{\phi_k} \prod_{j<m} f(r_{jm}) \\
&\quad + \prod_i g(\alpha,\beta,\mathbf{r}_i) \prod_{j<m} f(r_{jm}) \sum_{l\neq k} \nabla_k u_{kl} \\
&= \left(\frac{\nabla_k \phi_k}{\phi_k} + \sum_{l\neq k} \nabla_k u_{kl} \right) \Psi_T(\mathbf{r})
\end{aligned} \tag{20}
$$

Next, we find the second derivative;

$$
\begin{aligned}
\frac{1}{\Psi_T(\mathbf{r})} \nabla_k^2 \Psi_T(\mathbf{r}) &= \frac{1}{\Psi_T(\mathbf{r})} \nabla_k \left(\left(\frac{\nabla_k \phi_k}{\phi_k} + \sum_{l\neq k} \nabla_k u_{kl} \right) \Psi_T(\mathbf{r}) \right) \\
&= \frac{1}{\Psi_T(\mathbf{r})} \left(\left(\phi_k \nabla_k \frac{1}{\phi_k} + \frac{\nabla_k^2 \phi_k}{\phi_k} + \sum_{l\neq k} \nabla_k^2 u_{kl} \right) \Psi_T(\mathbf{r}) + \left(\frac{\nabla_k \phi_k}{\phi_k} + \sum_{l\neq k} \nabla_k u_{kl} \right)^2 \Psi_T(\mathbf{r}) \right) \\
&= \left(\frac{\nabla_k \phi_k}{\phi_k} \right)^2 + \frac{\nabla_k^2 \phi_k}{\phi_k} + \sum_{l\neq k} \nabla_k^2 u_{kl} + \left(\frac{\nabla_k \phi_k}{\phi_k} + \sum_{l\neq k} \nabla_k u_{kl} \right)^2 \\
&= -\left(\frac{\nabla_k \phi_k}{\phi_k} \right)^2 + \frac{\nabla_k^2 \phi_k}{\phi_k} + \sum_{l\neq k} \nabla_k^2 u_{kl} + \left(\frac{\nabla_k \phi_k}{\phi_k} \right)^2 + 2 \left(\frac{\nabla_k \phi_k}{\phi_k} \sum_{l\neq k} \nabla_k u_{kl} \right) + \left(\sum_{l\neq k} \nabla_k u_{kl} \right)^2 \\
&= \frac{\nabla_k^2 \phi_k}{\phi_k} + 2 \frac{\nabla_k \phi_k}{\phi_k} \sum_{l\neq k} \nabla_k u_{kl} + \sum_{l\neq k} \nabla_k^2 u_{kl} + \left(\sum_{l\neq k} \nabla_k u_{kl} \right)^2
\end{aligned} \tag{21}
$$

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;

$$\begin{aligned}
\frac{1}{\Psi_T(\mathbf{r})} \nabla_k^2 \Psi_T(\mathbf{r}) = & \frac{\nabla_k^2 \phi_k}{\phi_k} + 2 \frac{\nabla_k \phi_k}{\phi_k} \sum_{l \neq k} \frac{\boldsymbol{r}_k - \boldsymbol{r}_l}{r_{kl}} u'_{kl} \\
& + \left(\sum_{l \neq k} \frac{\boldsymbol{r}_k - \boldsymbol{r}_l}{r_{kl}} \partial u'_{kl}\right)^2 \\
& + \sum_{l \neq k} \left(\frac{d-1}{r_{kl}} u'_{kl} + u''_{kl}\right)
\end{aligned} \tag{22}$$

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

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

3 Results

4 Conclusions

References

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

Appendices

Appendix 1.