PHY635, I-Semester 2019/20, Assignment 1, solution

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(1) Many body wave functions: Translate the following sentences into math, i.e. write down the described quantum many-body states. For each first assume the particles are distinguishable, then also specify the wave function for indistinguishable Bosons or Fermions. In each case, make a 2D contour drawing of the wave-functions. [8 points]:

(i) One is in the ground-state of the harmonic oscillator, and another has momentum $p_0 > 0$.

(ii) Two particles of mass M are bound to each other, with a wave-function the modulus of which drops of as $\exp[-r/\xi]$ with separation r between them. The compound object created has momentum p_0.

(iii) Particle one is localized with Gaussian shape and width σ_1 near x_a. Particle two near x_b with width σ_2.

(iv) The same as in (iii), for $x_a = x_b = 0$ and $\sigma_1 = \sigma_2 = \sigma$, but due to some interactions, the particles avoid each other, such that the probability to find them a distance r apart drops of as $p(r) \sim \tanh(r/\xi)^2$, with $\xi \ll \sigma_{1,2}$

Solution:

(i) The two-body wave-function of the particle when they are distinguishable is:

$$\Psi_{dis}(x_1, x_2) = \psi_1(x_1)\psi_2(x_2), \tag{1}$$

where $\psi_1(x_1) = \frac{1}{\sqrt{\sqrt{\pi}\sigma}} \exp\left(-\frac{x_1^2}{2\sigma^2}\right)$ *and* $\psi(x_2) = \exp\left(\frac{-ip_0x_2}{\hbar}\right)$ *are the single-particle wave-function of particle 1 at position* x_1 *and particle 2 at position* x_2 *respectively. Putting the expression of* $\psi_1(x_1)$ *and* $\psi_2(x_2)$ *the two-body wave-function is:*

$$\Psi_{dis}(x_1, x_2) = \frac{1}{\sqrt{\sqrt{\pi}\sigma}} \exp\left(-\frac{x_1^2}{2\sigma^2}\right) \exp\left(\frac{-ip_0x_2}{\hbar}\right) \tag{2}$$

If the two particles are indistinguishable, then the two-body wave-function is:

$$\begin{aligned}
\Psi_{indis}(x_1, x_2) &= [\psi_1(x_1)\psi_2(x_2) \pm \psi_1(x_2)\psi_2(x_1)]/\sqrt{2} && (3)\\
&= \left[\frac{1}{\sqrt{\sqrt{\pi}\sigma}} \exp\left(-\frac{x_1^2}{2\sigma^2}\right) \exp\left(\frac{-ip_0x_2}{\hbar}\right)\right. && (4)\\
&\left.\pm \frac{1}{\sqrt{\sqrt{\pi}\sigma}} \exp\left(\frac{x_2^2}{2\sigma^2}\right) \exp\left(\frac{-ip_0x_1}{\hbar}\right)\right]\sqrt{2}, && (5)
\end{aligned}$$

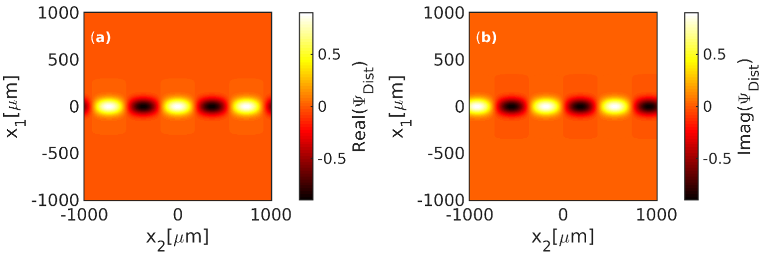

Fig. 1. [For part (i)] Panel (a) and (b) is the real and imaginary part of the wave-function for the distinguishable particles.

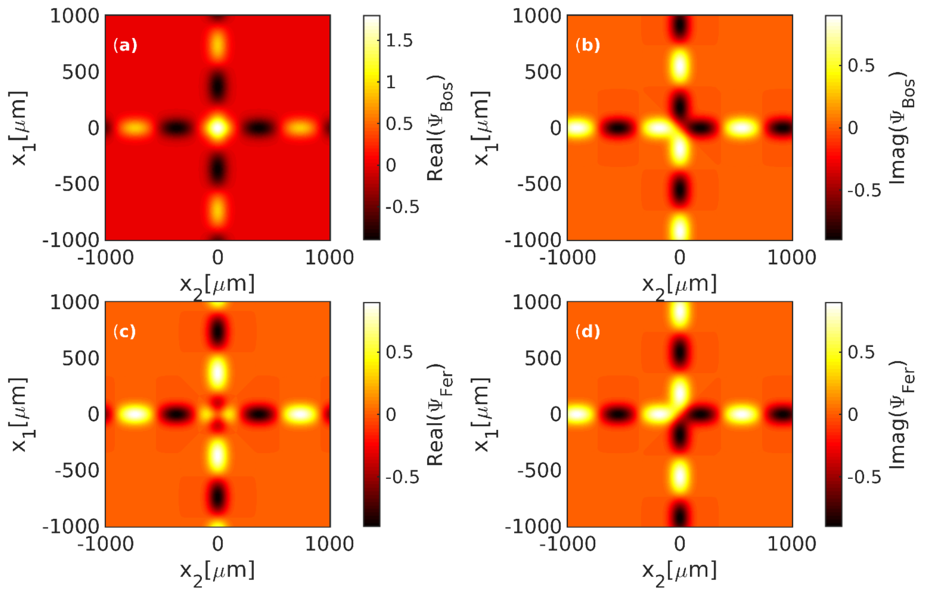

Fig. 2. [For part (i)] Panel (a) and (b) are the real and imaginary parts of the wave-function for Bosons. Panel (c) and (d) are the real and imaginary parts of the wave-function for the Fermions.

where $+$ and $-$ is for Bosons and Fermions respectively. The respective 2D plots of the wave-function for distinguishable and indistinguishable are shown in Fig. 1 and Fig. 2.

(ii) Since no specific information is given about either particle, we can skip the distinguishable case here. The wave-function of the two-body system can be written as:

$$\Psi_{dis}(x_1, x_2) = \mathcal{N} \exp\left(- \frac{|x_1 - x_2|}{\xi} \right) \exp\left[ip_0(x_1 + x_2)/(2\hbar)\right], \tag{6}$$

where $\mathcal{N}$ is a normalisation factor set to one in the following. This is completely symmetric under $x_1 \leftrightarrow x_2$. It turns out this form cannot be easily converted to be anti-symmetric for Fermions, so we skip that case here as well. The result for Bosons is shown in Fig. 3.

(iii) The two-body wave-function for the distinguishable particles localized with Gaussian

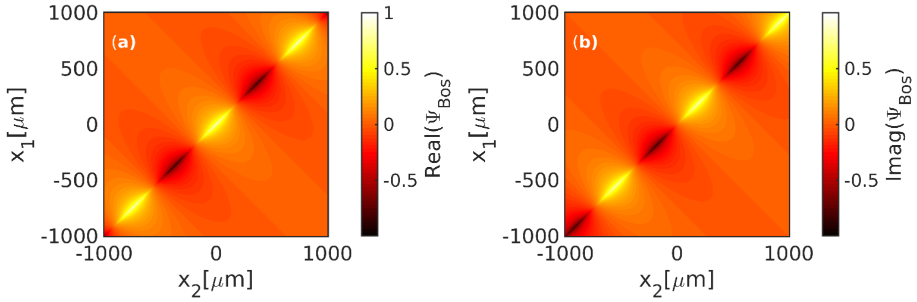

Fig. 3. [For part (ii)] Panel (a) and (b) are the wave-functions for the Bosonic and Fermionic nature of the particles in the limit $\xi \ll |x_a - x_b|$ respectively. Panel (c) and (d) are the wave-functions for the Bosons and Fermions in the limit $\xi \approx |x_a - x_b|$ respectively.

shape is:

$$\Psi_{dis}(x_1, x_2) = \frac{1}{\sqrt{\sqrt{\pi}\sigma_1}} \exp\left(-\frac{(x_1 - x_a)^2}{2\sigma_2^2}\right) \frac{1}{\sqrt{\sqrt{\pi}\sigma_2}} \exp\left(-\frac{(x_2 - x_b)^2}{2\sigma_2^2}\right) \tag{7}$$

Similarly the two-body wave-function for the indistinguishable particles is:

$$\Psi_{indis}(x_1, x_2) = \left[\frac{1}{\sqrt{\sqrt{\pi}\sigma_1}} \exp\left(-\frac{(x_1 - x_a)^2}{2\sigma_1^2}\right) \frac{1}{\sqrt{\sqrt{\pi}\sigma_2}} \exp\left(-\frac{(x_2 - x_b)^2}{2\sigma_2^2}\right)\right. \tag{8}$$

$$\left. \pm \frac{1}{\sqrt{\sqrt{\pi}\sigma_1}} \exp\left(-\frac{(x_2 - x_a)^2}{2\sigma_1^2}\right) \frac{1}{\sqrt{\sqrt{\pi}\sigma_2}} \exp\left(-\frac{(x_1 - x_b)^2}{2\sigma_2^2}\right)\right] / \sqrt{2}, \tag{9}$$

where + and − is for Bosonic and Fermionic nature of the particles respectively. The respective 2D plots for the two cases is shown in Fig 5 and Fig 6 for different limits of the parameters ($\sigma_{1,2}$).

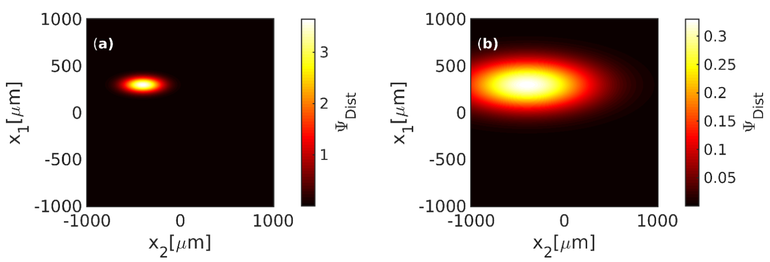

Fig. 4. [For part (iii)] Panel (a) and (b) are the wave-functions of the distinguishable particles for $\sigma_{1,2} \ll |x_a - x_b|$ and $\sigma_{1,2} \approx |x_a - x_b|$ respectively, where $x_a = 300\mu m$ and $x_b = -300\mu m$.

(iv) *Again, nothing in the text singles out an individual particle, so we directly go to indistinguishable ones, and could write*

$$\Psi(x_1, x_2) = \tanh\left(\frac{x_1 - x_2}{\xi}\right) \frac{1}{\sqrt{\pi\sigma^2}} \exp\left(-\frac{(x_1)^2}{2\sigma^2}\right) \exp\left(-\frac{(x_2)^2}{2\sigma^2}\right), \tag{10}$$

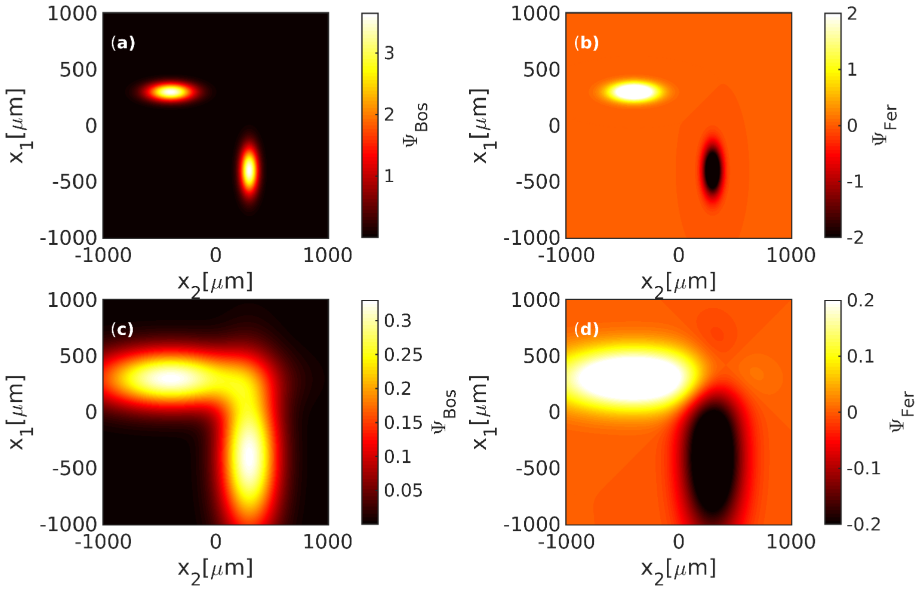

Fig. 5. [For part (iii)] Panel (a) and (b) are the wave-functions for the Bosons and Fermions in the limit $\sigma_{1,2} \ll |x_a - x_b|$ respectively. Panel (c) and (d) are the wave-functions for the Bosons and Fermions in the limit $\sigma_{1,2} \approx |x_a - x_b|$ respectively.

for Fermions and

$$\Psi(x_1, x_2) = \tanh\left(\frac{|x_1 - x_2|}{\xi}\right)\frac{1}{\sqrt{\pi\sigma^2}}\exp\left(-\frac{(x_1)^2}{2\sigma^2}\right)\exp\left(-\frac{(x_2)^2}{2\sigma^2}\right), \qquad (11)$$

for Bosons. The respective 2D plots for the two cases is shown in Fig 7 and Fig 8.

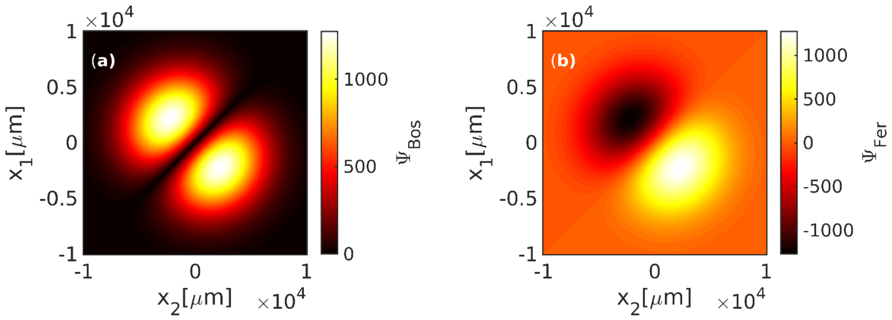

Fig. 6. [For part (iv)] Panel (a) Bosons, panel (b) Fermions.

(2) Ladder operators: Determine the following matrix elements for Bosonic operators/states in a three mode problem [6 points]

$$\mathcal{M}_1 = \langle\, 110\,|\hat{a}_2\hat{a}_2^\dagger\hat{a}_2^\dagger|\, 101\,\rangle, \qquad \mathcal{M}_2 = \langle\, 110\,|\hat{a}_2^\dagger\hat{a}_2^\dagger\hat{a}_2|\, 101\,\rangle,$$
$$\mathcal{M}_3 = \langle\, 113\,|\hat{a}_3^\dagger|\, 112\,\rangle, \qquad \mathcal{M}_4 = \langle\, 223\,|\hat{a}_2^\dagger|\, 113\,\rangle,$$
$$\mathcal{M}_5 = \langle\, 010\,|\hat{a}_2^\dagger\hat{a}_3|\, 001\,\rangle, \qquad \mathcal{M}_6 = \langle\, 302\,|\hat{a}_2\hat{a}_3^\dagger|\, 301\,\rangle. \qquad (12)$$

Determine the following matrix elements for Fermionic operators/states in a three mode problem [6 points]

$$\mathcal{M}_1 = \langle\, 110\,|\hat{a}_2\hat{a}_2^\dagger\hat{a}_2^\dagger|\,101\,\rangle, \qquad \mathcal{M}_2 = \langle\, 110\,|\hat{a}_2\hat{a}_2^\dagger\hat{a}_2^\dagger\hat{a}_2|\,110\,\rangle,$$
$$\mathcal{M}_3 = \langle\, 110\,|\hat{a}_1^\dagger\hat{a}_1\hat{a}_3\hat{a}_3^\dagger|\,110\,\rangle, \qquad \mathcal{M}_4 = \langle\, 001\,|\hat{a}_2\hat{a}_3^\dagger|\,010\,\rangle,$$
$$\mathcal{M}_5 = \langle\, 010\,|\hat{a}_2^\dagger\hat{a}_3|\,001\,\rangle, \qquad \mathcal{M}_6 = \langle\, 101\,|\hat{a}_2\hat{a}_3^\dagger|\,001\,\rangle. \tag{13}$$

Solution: *The matrix elements for the Bosonic operators/states are:*

$$\mathcal{M}_1 = 0, \mathcal{M}_2 = 0,$$
$$\mathcal{M}_3 = \sqrt{3}, \mathcal{M}_4 = 0,$$
$$\mathcal{M}_5 = 1, \mathcal{M}_6 = 0. \tag{14}$$

The matrix elements for the Fermionic operators/states are:

$$\mathcal{M}_1 = 0, \mathcal{M}_2 = 0,$$
$$\mathcal{M}_3 = 1, \mathcal{M}_4 = 0,$$
$$\mathcal{M}_5 = 1, \mathcal{M}_6 = 0. \tag{15}$$

(3) Hamiltonian in second quantisation: Consider a multi-electron atom such as Uranium, let us say N_e electrons. The Hamiltonian in atomic units is

$$\hat{H} = \sum_{i=1}^{N_e}\left(-\frac{1}{2}\nabla^2_{\mathbf{r}_i} - \frac{Z}{r_i}\right) + \sum_{i<j=1}^{N_e}\frac{1}{r_{ij}}, \tag{16}$$

where $\mathbf{r}_j$ is the position of electron j relative to the nucleus, $r_j = |\mathbf{r}_j|$ and $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ and Z the nuclear charge. Use the single particle basis of spin-less Hydrogenic states $|\,\varphi_{nlm}\,\rangle$ fulfilling $\hat{H}_Z|\,\varphi_{nlm}\,\rangle = E_n|\,\varphi_{nlm}\,\rangle$ with $\hat{H}_Z = -\frac{1}{2}\nabla^2_{\mathbf{r}} - \frac{Z}{r}$ and associated Fermionic creation operators $\hat{a}_{nlm}$, to convert that Hamiltonian into a second quantized form [10 points].

Solution: *The given Hamiltonian can be written as:*

$$\hat{H} = \sum_{i=1}^{N_e}(\hat{H}_Z)_i + \sum_{i<j=1}^{N_e}\hat{U}_{ij}, \tag{17}$$

where $(H_Z)_i = \frac{1}{2}\nabla^2_{\mathbf{r}_i} - \frac{Z}{r_i}$ is the single electron Hamiltonian and $U_{ij} = \frac{1}{r_{ij}}$ is the interaction between the electrons.

Using Eq 2.13 from the lecture notes, the second quantized Hamiltonian in Hydrogenic state ($|\,\psi_{nlm}\,\rangle$) can be written as:

$$\hat{H} = \sum_{nlm,n'l'm'} A_{nlm,n'l'm'}\hat{a}^\dagger_{nlm}\hat{a}_{n'l'm'} + \sum_{nlm,n'l'm'}\sum_{rst,r's't'} B_{nlm,n'l'm'rst,r's't'}\hat{a}^\dagger_{nlm}\hat{a}^\dagger_{n'l'm'}\hat{a}_{rst}\hat{a}_{r's't'}, \tag{18}$$

where

$$A_{nlm,n'l'm'} = \langle\, \psi_{nlm}\, |H_Z|\, \psi_{n'l'm'}\, \rangle = E_n \langle\, \psi_{nlm}\, ||\, \psi_{n'l'm'}\, \rangle = E_n \delta_{nn'} \delta_{ll'} \delta_{mm'} \tag{19}$$

and

$$\begin{aligned} B_{nlm,n'l'm',rst,r's't'} &= \langle\, \psi_{nlm}\psi_{n'l'm'}\, |\hat{U}_{ij}|\, \psi_{rst}\psi_{r's't'}\, \rangle \\ &= \int d\mathbf{r}_i \int d\mathbf{r}_j \psi^*_{nlm}(\mathbf{r}_i)\psi^*_{n'l'm'}(\mathbf{r}_j) U(\mathbf{r}_i, \mathbf{r}_j)\psi_{rst}(\mathbf{r}_i)\psi_{r's't'}(\mathbf{r}_j), \end{aligned} \tag{20}$$

which cannot easily be evaluated explicitly.
Putting the value of $A_{nlmn'l'm'}$ and $B_{nlmn'l'm'rstr's't'}$ in second quantized Hamiltonian we get:

$$\hat{H} = \sum_{nlm} E_n \hat{a}^\dagger_{nlm} \hat{a}_{nlm} + \sum_{nlm,n'l'm'} \sum_{rst,r's't'} B_{nlm,n'l'm',rst,r's't'} \hat{a}^\dagger_{nlm} \hat{a}^\dagger_{n'l'm'} \hat{a}_{rst} \hat{a}_{r's't'} \tag{21}$$

(4) Numerical Quantum Many Body Physics Consider two coupled quantum mechanical harmonic oscillators of mass $m = 1$ and frequency $\omega = 1$, described with the first quantized Hamiltonian

$$H = \frac{1}{2}\left(p_1^2 + x_1^2\right) + \frac{1}{2}\left(p_2^2 + x_2^2\right) + 2\kappa x_1 x_2, \tag{22}$$

where x_i is the position of oscillator i and p_i its momentum.

(4a) Write down the corresponding two-body Schrödinger equation for a wave function $\Psi(x_1, x_2)$ in the position space representation. You may treat the oscillators as distinguishable. [3 points]

(4b) In terms of $\Psi(x_1, x_2)$, also derive expressions for the energy expectation value, and split it into energy of oscillator 1, energy of oscillator 2 and interaction energy. [2 points]

(4c) Edit the template file `Assignment1_phy635_program_draft_v1.xmds` provided online. It presently contains the Schrödinger equation and energy sampling as appropriate when particle 1 is a free particle and particle 2 is ignored. Edit this to include your results from (4a), (4b). [1 points]

(4d) Implement as initial condition for the wave function $\Psi(x_1, x_2) = \frac{1}{\sqrt{\sqrt{\pi}\sigma}} \exp\left(-\frac{x_1^2}{2\sigma^2}\right) \frac{x_2\sqrt{2}}{\sigma\sqrt{\sqrt{\pi}\sigma}} \exp\left(-\frac{x_2^2}{2\sigma^2}\right)$, and convince yourself that this corresponds to oscillator 1 in the ground state and oscillator 2 in the excited state. Follow the info-sheet `Numerics_assignments_info.pdf` to run your code until time $t_{fin} = 100$ once implemented. First, check that normalization and total energy are conserved, using `Assignment1_plot_checks_v1.m`. Then check the individual energy components using `Assignment1_plot_energies_v1.m`. Discuss your results. Also inspect the actual evolution of the many-body density using `Assignment1_density_slideshow_v1.m`, and comment on that as well. [4 points]

Solution:

(4a)

The given Hamiltonian can also be written as:

$$\hat{H} = \sum_{i=1}^{2} \frac{(\hat{p}_i^2 + \hat{x}_i^2)}{2} + k \sum_{i<j=1}^{2} \hat{x}_i \hat{x}_j$$

$$= \sum_{i=1}^{2} (\hat{H}_0)_i + \sum_{i<j=1}^{2} \hat{U}_{i,j}, \tag{23}$$

where $(\hat{H}_0)_i = \frac{(\hat{p}_i^2 + \hat{x}_i^2)}{2}$ *and* $\hat{U}_{i,j} = k\hat{x}_i\hat{x}_j$ *is the single oscillator Hamiltonian and interaction between the oscillators respetively.*

The Schrödinger equation for $\Psi(x_1, x_2)$ *is given as:*

$$i\hbar \frac{d\Psi(x_1, x_2)}{dt} = \hat{H}\Psi(x_1, x_2)$$

$$= \left(\sum_{i=1}^{2} \frac{(\hat{p}_i^2 + \hat{x}_i^2)}{2} + k \sum_{i<j=1}^{2} \hat{x}_i \hat{x}_j \right) \Psi(x_1, x_2). \tag{24}$$

(4b) Assuming the particles are distinguishable, the two-body wave-function can be written as:

$$\Psi(x_1, x_2) = \psi(x_1)\phi(x_2). \tag{25}$$

Now the expectation value of energy is given by:

$$E = \langle\, \Psi(x_1, x_2)\, |\hat{H}|\, \Psi(x_1, x_2)\, \rangle$$

$$= \int dx_1 \int dx_2 \Psi^*(x_1, x_2) H \Psi(x_1, x_2)$$

$$= \int dx_1 \int dx_2 \Psi^*(x_1, x_2) \frac{(p_1^2 + x_1^2)}{2} \Psi(x_1, x_2) + \int dx_1 \int dx_2 \Psi^*(x_1, x_2) \frac{(p_2^2 + x_2^2)}{2} \Psi(x_1, x_2)$$

$$+ 2k \int dx_1 \int dx_2 \Psi^*(x_1, x_2) \{x_1 x_2\} \Psi(x_1, x_2) \tag{26}$$

The first and second term is the energy of the oscillator 1 and oscillator 2 respectively and the last term is the interaction energy.

(4d)

If particle 1 is in the ground state and particle 2 is in the first excited state of the harmonic oscillator, then the two-body wavefunction is:

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{\sqrt{\pi}\sigma}} \exp\left(-\frac{x_1^2}{2\sigma^2} \right) \frac{x_2\sqrt{2}}{\sigma\sqrt{\sqrt{\pi}\sigma}} \exp\left(-\frac{x_2^2}{2\sigma^2} \right) \tag{27}$$

The individual energy components and the density of two-body system is shown in Fig 9 and Fig 10.

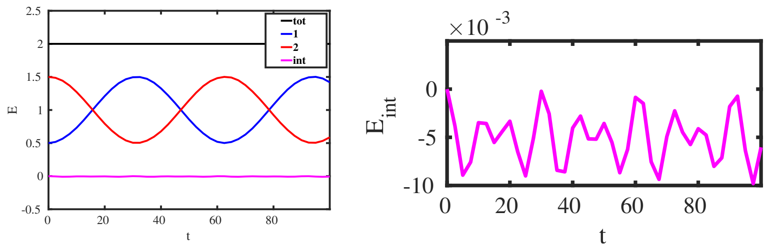

Fig. 7. (left) Decomposition of total energy (black lines) of the two-body system into energy of particle 1 (blue lines) and particle 2 (red lines). (right) Note that the interaction energy (pink lines) given by Eq. (26) remains small, $E_{\rm int} \approx 0.01$, yet is responsible for the energy exchange between the two oscillators.

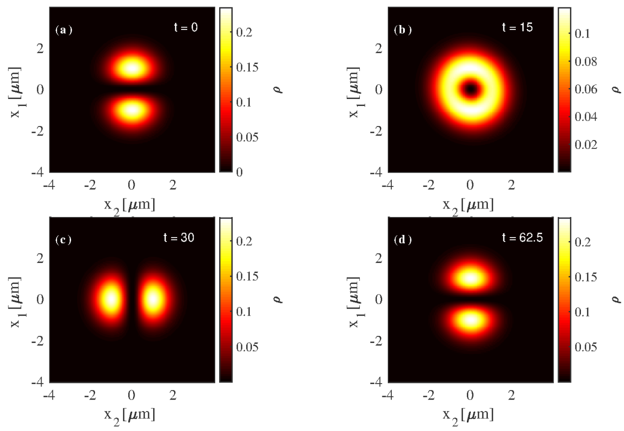

Fig. 8. A few different time samples of the two-body density. Panel (a) is the intial state of the two-body system in which particle 1 is in the ground state and particle 2 is in the excited state of the harmonic oscillator. Panel (b) shows the equal probability of the two-particle being in either state of the harmonic oscillator. The particles have swapped states at t = 30, as shown in panel (c) and again come back to the original state, as shown in panel (d). Compare with Fig. 7.