## PHY635, II-Semester 2022/23, Assignment 1 solution

(1) Two-body wave functions: Consider two particles in one dimension, one at position $r_{1}$ and the other at $r_{2}$. Translate the following sentences into math, i.e. write down the described quantum many-body states. For each first assume the two particles are distinguishable, then also specify the wave function for indistinguishable Bosons or Fermions. In each case, make a 2 D contour drawing in the space $\left(r_{1}, r_{2}\right)$ of the wave-functions, indicating signs or Re and Im as well. [6 points]:
(a) One is in the $n=1$ state of the harmonic oscillator, and the other in $n=2$.
(b) Neutron A is stuck in a nucleus between $r_{1}=0$ and $r_{2}=R$ in its ground-state, while neutron B impinges on the nucleus from negative $r_{2}$ and elastically scatters off it in the backwards direction.
(c) Particle A is localized with Gaussian wavefunction and width $\sigma_{A}$ near $x_{A}$. Particle B near $x_{B}$ with width $\sigma_{B}$. Compare the two cases (i) $\sigma_{A}=\sigma_{B}=\sigma \ll\left|x_{A}-x_{B}\right|$ and (ii) $\sigma_{A}=\sigma_{B}=\sigma \approx\left|x_{A}-x_{B}\right|$, separately for indistinguishable particles, Bosons and Fermions.

Solution: See Assignment1_solution.nb in numerics solution package.
(2) Creation and destruction operators:
(a) Let $\hat{a}_{k}$ be a fermionic destruction operator for a multi-mode system, with index $k$ numbering the mode. Find the simplest expression for the operator product

$$
\begin{equation*}
\hat{a}_{k}^{\dagger} \hat{a}_{\ell} \hat{a}_{\ell}^{\dagger} \hat{a}_{k}^{\dagger} \hat{a}_{k} \tag{1}
\end{equation*}
$$

and justify your answer [2ps].
Solution: We can write $\hat{a}_{k}^{\dagger} \hat{a}_{\ell} \hat{a}_{\ell}^{\dagger} \hat{a}_{k}^{\dagger} \hat{a}_{k}=0$. For $\ell=k$ we have

$$
\begin{equation*}
\hat{a}_{k}^{\dagger} \hat{a}_{k} \hat{a}_{k}^{\dagger} \hat{a}_{k}^{\dagger} \hat{a}_{k}=\frac{1}{2} \hat{a}_{k}^{\dagger} \hat{a}_{k}\left\{\hat{a}_{k}^{\dagger}, \hat{a}_{k}^{\dagger}\right\} \hat{a}_{k} \text { Eq. (2.8) } 0 \tag{2}
\end{equation*}
$$

otherwise

$$
\begin{align*}
& \hat{a}_{k}^{\dagger} \hat{a}_{\ell} \hat{a}_{\ell}^{\dagger} \hat{a}_{k}^{\dagger} \hat{a}_{k} \text { Eq. (2.8) } \\
& =\hat{a}_{k}^{\dagger} \hat{a}_{\ell} \hat{a}_{k}^{\dagger} \hat{a}_{\ell}^{\dagger} \hat{a}_{k}  \tag{3}\\
& \text { Eq. (2.8) } \hat{a}_{k}^{\dagger} \hat{a}_{k}^{\dagger} \hat{a}_{\ell} \hat{a}_{\ell}^{\dagger} \hat{a}_{k}=\frac{1}{2}\left\{\hat{a}_{k}^{\dagger}, \hat{a}_{k}^{\dagger}\right\} \hat{a}_{\ell} \hat{a}_{\ell}^{\dagger} \hat{a}_{k}=0
\end{align*}
$$

(b) Consider a bosonic two-mode problem, with $\hat{a}, \hat{b}$ the destruction operator for the two modes, and $|n, m\rangle$ the Fock states describing them. We define the operators $\hat{C}=\hat{a}^{\dagger} \hat{a}+\hat{b}^{\dagger} \hat{b}, \hat{D}=\hat{a}^{\dagger} \hat{a}-\hat{b}^{\dagger} \hat{b}$. First give a physical interpretation of both. Then write the most general separable two-mode state, compare the variance of $\hat{C}$ and $\hat{D}$ and discuss [2pts].

Solution: Since $\hat{N}_{a}=\hat{a}^{\dagger} \hat{a}\left(\hat{N}_{b}=\hat{b}^{\dagger} \hat{b}\right)$ is the operator for the Boson number in mode $A(B)$, we can see that $\hat{C}$ is the operator for the total number of Bosons combining both modes, and $\hat{D}$ for the number difference between the two modes. The most general state for either mode can be written as e.g. $\left|\psi_{a}\right\rangle=\sum_{n=0}^{\infty} c_{n}|n\rangle$ and $\left|\psi_{b}\right\rangle=$ $\sum_{m=0}^{\infty} d_{m}|m\rangle$, thus the most general separable two-mode state is

$$
\begin{equation*}
|\Psi\rangle=\left|\psi_{a}\right\rangle \otimes\left|\psi_{b}\right\rangle=\sum_{n m} c_{n} d_{m}|n, m\rangle, \tag{4}
\end{equation*}
$$

where $\sum_{n}\left|c_{n}\right|^{2}=\sum_{m}\left|d_{m}\right|^{2}=1$.
We can write the variances as

$$
\begin{equation*}
\operatorname{Var}[\hat{C} \text { or } \hat{D}]=\left\langle\left(\hat{N}_{a} \pm \hat{N}_{b}\right)^{2}\right\rangle-\left\langle\left(\hat{N}_{a} \pm \hat{N}_{b}\right)^{2}\right\rangle^{2} \tag{5}
\end{equation*}
$$

as usual, where we have "+" for $\hat{C}$ and "-" for $\hat{D}$. Expanding the squares

$$
\begin{equation*}
=\langle\hat{N}_{a}^{2}+\hat{N}_{b}^{2} \pm 2 \underbrace{\hat{N}_{a} \hat{N}_{b}}_{\langle\cdots\rangle=\left\langle\hat{N}_{a}\right\rangle\left\langle\hat{N}_{b}\right\rangle}\rangle-\left[\left\langle\left(\hat{N}_{a}\right\rangle^{2}+\left\langle\hat{N}_{b}\right\rangle^{2} \pm 2\left\langle\hat{N}_{a}\right\rangle\left\langle\hat{N}_{b}\right\rangle\right]\right. \tag{6}
\end{equation*}
$$

For the expression at $\underbrace{\ldots}$ we used that the expectation value in the separable state must factor, which you can also explicitly verify with the coefficients given above. Thus the $\pm$ terms cancel and we can group the rest into:

$$
\begin{equation*}
=\underbrace{\left\langle\hat{N}_{a}^{2}\right\rangle-\left\langle\left(\hat{N}_{a}\right)^{2}\right.}_{\equiv \operatorname{Var}\left[\hat{N}_{a}\right]}+\underbrace{\left\langle\hat{N}_{b}^{2}\right\rangle-\left\langle\left(\hat{N}_{b}\right\rangle^{2}\right.}_{\equiv \operatorname{Var}\left[\hat{N}_{b}\right]} \tag{7}
\end{equation*}
$$

Thus the two variances of $C$ and $D$ are equal to each other and equal to the sum of the number variances for mode $A$ and $B$. This is only true for the given separable state, so if these two deviate, the state must be entangled.
(3) Hamiltonian in second quantisation: Consider $N_{e}$ electrons in some external potential $V(\mathbf{x})$, for example the lattice potential of the ion crystal in a a solid material, interacting through Coulomb interactions with Hamiltonian:

$$
\begin{equation*}
\hat{H}=\sum_{i=1}^{N_{e}}\left(-\frac{\hbar^{2}}{2 m_{e}} \nabla_{\mathbf{r}_{i}}^{2}+V\left(\mathbf{r}_{i}\right)\right)+\sum_{i<j=1}^{N} \frac{e^{2}}{\left(4 \pi \epsilon_{0}\right)\left|\mathbf{r}_{i}-\mathbf{r}_{j}\right|}, \tag{8}
\end{equation*}
$$

where $\mathbf{r}_{j}$ is the position of electron $j$. Use the single particle basis $|\sigma, \mathbf{k}\rangle$, corresponding to an electron with spin (z-component) $\sigma \in\{\uparrow, \downarrow\}$ and wavenumber $\mathbf{k}$ to convert Eq. (8) into a second quantised Hamiltonian, for operators $\hat{a}_{\sigma \mathbf{k}}\left(\hat{a}_{\sigma \mathbf{k}}^{\dagger}\right)$. Use box-quantised plane wave states, i.e. $\langle\mathbf{x} \mid \sigma, \mathbf{k}\rangle=\frac{1}{\sqrt{\nu}} e^{i \mathbf{k} \cdot \mathbf{x}} \xi_{\sigma}$, where $\xi_{\sigma}$ is a spinor. Discuss each term in your Hamiltonian, what is physically implies, why it takes the form it takes, and what conservation laws might be encoded in it. [10 points].
Solution: We identify that the Hamiltonian contains single body and two-body terms.

Generalising Eq. (2.14) of the lecture to one continuous wavenumber index and one discrete spin index, we should in principle start out with:

$$
\begin{align*}
\hat{H} & =\sum_{\sigma \sigma^{\prime}} \int d k \int d k^{\prime} A_{\sigma \sigma^{\prime}}\left(k, k^{\prime}\right) \hat{a}_{\sigma \mathbf{k}}^{\dagger} \hat{a}_{\sigma^{\prime} \mathbf{k}^{\prime}} \\
& +\sum_{\sigma \sigma^{\prime} \sigma^{\prime \prime} \sigma^{\prime \prime \prime}} \int d k \int d k^{\prime} \int d k^{\prime \prime} \int d k^{\prime \prime \prime \prime} B_{\sigma \sigma^{\prime} \sigma^{\prime \prime} \sigma^{\prime \prime \prime}}\left(k, k^{\prime}, k^{\prime \prime}, k^{\prime \prime \prime}\right) \hat{a}_{\sigma \mathbf{k}}^{\dagger} \hat{a}_{\sigma^{\prime} \mathbf{k}^{\prime}}^{\dagger} \hat{a}_{\sigma^{\prime \prime} \mathbf{k}^{\prime \prime}} \hat{a}_{\sigma^{\prime \prime \prime} \mathbf{k}^{\prime \prime \prime}} \tag{9}
\end{align*}
$$

Applying the recipe for the coefficients (2.15) to the single body terms gives us:

$$
\begin{equation*}
A_{\sigma \sigma^{\prime}}\left(k, k^{\prime}\right)=\langle\sigma, \mathbf{k}|\left[-\frac{\hbar^{2}}{2 m_{e}} \nabla_{\mathbf{x}}^{2}+V(\mathbf{x})\right]\left|\sigma^{\prime}, \mathbf{k}^{\prime}\right\rangle \tag{10}
\end{equation*}
$$

Nothing in $\hat{H}_{0}$ depends on the spin, so the scalar product of the spinors $\xi_{\sigma}^{*} \cdot \xi_{\sigma^{\prime}}=\delta_{\sigma \sigma^{\prime}}$. For the spatial part

$$
\begin{align*}
A_{\sigma \sigma^{\prime}}\left(k, k^{\prime}\right) & =\delta_{\sigma \sigma^{\prime}} \frac{1}{\mathcal{V}} \int d^{3} \mathbf{x} e^{-i \mathbf{k} \cdot \mathbf{x}}\left[-\frac{\hbar^{2}}{2 m_{e}} \nabla_{\mathbf{x}}^{2}+V(\mathbf{x})\right] e^{i \mathbf{k}^{\prime} \cdot \mathbf{x}} \\
& =\delta_{\sigma \sigma^{\prime}} \frac{1}{\mathcal{V}}\left[\mathcal{V} \delta_{\mathbf{k ^ { \prime }}}\left(\frac{\hbar^{2} \mathbf{k}^{\prime 2}}{2 m}\right)+\int d^{3} \mathbf{x} e^{-i\left(\mathbf{k}-\mathbf{k}^{\prime}\right) \cdot \mathbf{x}} V(\mathbf{x})\right]=\delta_{\sigma \sigma^{\prime}}\left[\delta_{\mathbf{k \mathbf { k } ^ { \prime }}}\left(\frac{\hbar^{2} \mathbf{k}^{\prime 2}}{2 m}\right)+\tilde{V}\left(\mathbf{k}-\mathbf{k}^{\prime}\right)\right] \tag{11}
\end{align*}
$$

where in the last step we have used the Fourier transform of the potential $\tilde{V}(\mathbf{k}) \equiv$ $\int d^{3} \mathbf{x} e^{-i \mathbf{k} \cdot \mathbf{x}} V(\mathbf{x}) / \mathcal{V}$.

For the two-body terms, we follow the same steps: [to be completed]

$$
\begin{equation*}
B_{\sigma \sigma^{\prime} \sigma^{\prime \prime} \sigma^{\prime \prime \prime}}\left(k, k^{\prime}, k^{\prime \prime}, k^{\prime \prime \prime}\right)=\left\langle\sigma, \mathbf{k} ; \sigma^{\prime}, \mathbf{k}^{\prime}\right| \frac{2 e^{2}}{\left(4 \pi \epsilon_{0}\right)|\mathbf{x}-\mathbf{y}|}\left|\sigma^{\prime \prime}, \mathbf{k}^{\prime \prime} ; \sigma^{\prime \prime \prime}, \mathbf{k}^{\prime \prime \prime}\right\rangle \tag{12}
\end{equation*}
$$

Again nothing depends on spin, giving us Kronecker deltas for the spin indices of the first and second particle.

$$
\begin{equation*}
B_{\sigma \sigma^{\prime} \sigma^{\prime \prime} \sigma^{\prime \prime \prime}}\left(k, k^{\prime}, k^{\prime \prime}, k^{\prime \prime \prime}\right)=\delta_{\sigma \sigma^{\prime \prime}} \delta_{\sigma^{\prime} \sigma^{\prime \prime \prime}} \frac{1}{\mathcal{V}^{2}} \int d^{3} \mathbf{x} \int d^{3} \mathbf{y} e^{-i \mathbf{k} \cdot \mathbf{x}} e^{-i \mathbf{k}^{\prime} \cdot \mathbf{y}} \frac{2 e^{2}}{\left(4 \pi \epsilon_{0}\right)|\mathbf{x}-\mathbf{y}|} e^{i \mathbf{k}^{\prime \prime} \cdot \mathbf{x}} e^{i \mathbf{k}^{\prime \prime \prime} \cdot \mathbf{y}} \tag{13}
\end{equation*}
$$

Let us change integration variables to $\mathbf{r}=(\mathbf{x}-\mathbf{y}) / 2$ and $\mathbf{R}=(\mathbf{x}+\mathbf{y}) / 2$, then (Warning: The following is not as cosmetically neat as possible and has various uncertaint factors of 2, but it should get the gist of the procedure across. I will enlist the help of some of you to polish the solution up )

$$
\begin{align*}
& B_{\sigma \sigma^{\prime} \sigma^{\prime \prime} \sigma^{\prime \prime \prime}}\left(k, k^{\prime}, k^{\prime \prime}, k^{\prime \prime \prime}\right)=\delta_{\sigma \sigma^{\prime \prime}} \delta_{\sigma^{\prime} \sigma^{\prime \prime \prime}} \frac{e^{2}}{4 \pi \epsilon_{0} \mathcal{V}^{2}} \int d^{3} \mathbf{r} \int d^{3} \mathbf{R} e^{-i \mathbf{k} \cdot[\mathbf{R}+\mathbf{r}]} e^{-i \mathbf{k}^{\prime} \cdot[\mathbf{R}-\mathbf{r}]} \frac{1}{|\mathbf{r}|} e^{i \mathbf{k}^{\prime \prime} \cdot[\mathbf{R}+\mathbf{r}]} e^{i \mathbf{k}^{\prime \prime \prime} \cdot[\mathbf{R}-\mathbf{r}]} \\
& =\delta_{\sigma \sigma^{\prime \prime}} \delta_{\sigma^{\prime} \sigma^{\prime \prime \prime}} \frac{e^{2}}{4 \pi \epsilon_{0} \mathcal{V}^{2}} \int d^{3} \mathbf{r} \underbrace{\int d^{3} \mathbf{R} e^{i\left(\mathbf{k}^{\prime \prime}+\mathbf{k}^{\prime \prime \prime}-\mathbf{k}-\mathbf{k}^{\prime}\right) \cdot \mathbf{R}} e^{-i\left(\mathbf{k}+\mathbf{k}^{\prime \prime \prime}-\mathbf{k}^{\prime}-\mathbf{k}^{\prime \prime}\right) \cdot \mathbf{r}} \frac{1}{|\mathbf{r}|}}_{=\mathcal{V} \delta\left(\mathbf{k}+\mathbf{k}^{\prime}-\mathbf{k}^{\prime \prime}-\mathbf{k}^{\prime \prime \prime}\right)} \tag{14}
\end{align*}
$$

The delta-function enforces $\mathbf{k}+\mathbf{k}^{\prime}=\mathbf{k}^{\prime \prime}+\mathbf{k}^{\prime \prime \prime}$, i.e. momentum conservation during the collision. Hence we must have: $\mathbf{k}=\mathbf{k}^{\prime \prime}+\mathbf{q} / 2$ with $\mathbf{k}^{\prime}=\mathbf{k}^{\prime \prime \prime}-\mathbf{q} / 2$ defining some momentum transfer $\mathbf{q}$. Using that definition in the second exponential we now have:
where we now have expressed everything in terms of the Fourier-transform of the interaction potential, wrt. the momentum transfer.

Insertion of single and two-body operators into the original (16) and using deltas etc. provides:

$$
\begin{align*}
\hat{H} & =\sum_{\sigma}\left[\int d k \frac{\hbar^{2} \mathbf{k}^{2}}{2 m} \hat{a}_{\sigma \mathbf{k}}^{\dagger} \hat{a}_{\sigma \mathbf{k}}+\int d k \int d k^{\prime} \tilde{V}\left(\mathbf{k}-\mathbf{k}^{\prime}\right) \hat{a}_{\sigma \mathbf{k}}^{\dagger} \hat{a}_{\sigma \mathbf{k}^{\prime}}\right] \\
& +\sum_{\sigma \sigma^{\prime}} \int d k \int d k^{\prime} \int d k^{\prime \prime} \int d k^{\prime \prime \prime \prime} \frac{e^{2}}{4 \pi \epsilon_{0}} \delta\left(\mathbf{k}+\mathbf{k}^{\prime}-\mathbf{k}^{\prime \prime}-\mathbf{k}^{\prime \prime \prime}\right) \tilde{V}(\mathbf{q}) \hat{a}_{\sigma \mathbf{k}}^{\dagger} \hat{a}_{\sigma^{\prime} \mathbf{k}^{\prime}}^{\dagger} \hat{a}_{\sigma \mathbf{k}^{\prime \prime}} \hat{a}_{\sigma^{\prime} \mathbf{k}^{\prime \prime \prime}} \\
& =\sum_{\sigma}\left[\int d k \frac{\hbar^{2} \mathbf{k}^{2}}{2 m} \hat{a}_{\sigma \mathbf{k}}^{\dagger} \hat{a}_{\sigma \mathbf{k}}+\int d k \int d k^{\prime} \tilde{V}\left(\mathbf{k}-\mathbf{k}^{\prime}\right) \hat{a}_{\sigma \mathbf{k}}^{\dagger} \hat{a}_{\sigma \mathbf{k}^{\prime}}\right] \\
& +\sum_{\sigma \sigma^{\prime}} \int d k \int d k^{\prime} \int d k^{\prime \prime} \frac{e^{2}}{4 \pi \epsilon_{0}} \tilde{V}(\mathbf{q}) \hat{a}_{\sigma \mathbf{k}}^{\dagger} \hat{a}_{\sigma^{\prime} \mathbf{k}^{\prime}}^{\dagger} \hat{\sigma}_{\sigma \mathbf{k}^{\prime \prime}} \hat{a}_{\sigma^{\prime}\left(\mathbf{k}+\mathbf{k}^{\prime}-\mathbf{k}^{\prime \prime}\right)} \tag{16}
\end{align*}
$$

Finally changing variables in the last integration from $\mathbf{k}^{\prime \prime}$ to $\mathbf{k}-\mathbf{q} / 2$ such that $\int^{3} d \mathbf{k}^{\prime \prime} \rightarrow$ $-\int^{3} d \mathbf{q} / 2$ we have (more factors of 2 and minus signs? )

$$
\begin{align*}
\cdots & =\sum_{\sigma}\left[\int d k \frac{\hbar^{2} \mathbf{k}^{2}}{2 m} \hat{a}_{\sigma \mathbf{k}}^{\dagger} \hat{a}_{\sigma \mathbf{k}}+\int d k \int d k^{\prime} \tilde{V}\left(\mathbf{k}-\mathbf{k}^{\prime}\right) \hat{a}_{\sigma \mathbf{k}}^{\dagger} \hat{a}_{\sigma \mathbf{k}^{\prime}}\right] \\
& +\sum_{\sigma \sigma^{\prime}} \int d k \int d k^{\prime} \int d q \frac{e^{2}}{4 \pi \epsilon_{0}} \tilde{V}(\mathbf{q}) \hat{a}_{\sigma \mathbf{k}}^{\dagger} \hat{a}_{\sigma^{\prime} \mathbf{k}^{\prime}}^{\dagger} \hat{a}_{\sigma(\mathbf{k}-\mathbf{q} / 2)} \hat{a}_{\sigma^{\prime}(\mathbf{k}+\mathbf{q} / 2)} . \tag{17}
\end{align*}
$$

(For logical sense, we want to add the $\mathbf{q}$ to the outgoing momenta. We can do this simply by more integration range shifts [or smarter definition of $q$ to begin with])

Please see also second_quantization_note_v7_en.pdf in the .zip file, thanks to https://kato.issp.u-tokyo.ac.jp/kato/index-e.html's upload on his webpage, Eq. (88)-(90).

Discussion of terms: The first term is the kinetic energy. That is diagonal in wavenumber $\mathbf{k}$ and spin $\sigma$ hence the double sums/integrals collapse into single sums/integrals. This encodes momentum and spin conservation for the free particle. The second term is the external potential energy. This still conserves spin, since the potential was not spin dependent, but can cause a change of the momentum through application of a force. So here we get a double integral over wavenumbers (momenta). The interaction term in the final line allows particles to impart momentum onto each other in a collision, but cannot change their total momentum. This is ensured by the nature of the remaining
integrations and coefficients. Momentum transfer $\mathbf{q}$ has an amplitude set by the corresponding Fourier coefficient of the interaction potential. Each particle separately keeps its spin, since interactions do not depend on spin.
(4) Numerical Quantum Many Body Physics Consider two indistinguishable particles at $r_{1}$ and $r_{2}$ (either Fermions or Bosons), moving in one dimension and interacting with a Gaussian potential (for simplicity). Their Hamiltonian thus is:

$$
\begin{equation*}
\hat{H}=-\frac{\hbar^{2}}{2 m}\left(\frac{\partial^{2}}{\partial r_{1}^{2}}+\frac{\partial^{2}}{\partial r_{2}^{2}}\right)+A e^{-\frac{\left(r_{1}-r_{2}\right)^{2}}{2 S^{2}}} \tag{18}
\end{equation*}
$$

where $A$ is an interaction strength and $S$ an interaction range.
(4a) Find the two-body Schrödinger equation, then express everything in terms of a centre of mass (CM) coordinate $R=\left(r_{1}+r_{2}\right) / 2$ and a relative coordinate $r=r_{2}-r_{1}$, and show that if two separate Schrödinger equations for the CM and relative motion are fulfilled, the origial equation is fulfilled. For this use the Ansatz $\Psi\left(r_{1}, r_{2}, t\right)=\phi(r, t) \varphi(R, t)$ for the two-body wavefunction. Discuss how the centre of mass wavefunction $\varphi(R, t)$ evolves. [2 points] vspace 0.25 cm
Solution: In terms of the two-particle wavefunction $\psi\left(r_{1}, r_{2}, t\right)$ we have the TDSE:

$$
\begin{equation*}
i \hbar \frac{\partial}{\partial t} \psi\left(r_{1}, r_{2}, t\right)=\left[-\frac{\hbar^{2}}{2 m}\left(\frac{\partial^{2}}{\partial r_{1}^{2}}+\frac{\partial^{2}}{\partial r_{2}^{2}}\right)+A e^{-\frac{\left(r_{1}-r_{2}\right)^{2}}{2 S^{2}}}\right] \psi\left(r_{1}, r_{2}, t\right) \tag{19}
\end{equation*}
$$

Inserting the factorisation Ansatz $\Psi\left(r_{1}, r_{2}\right)=\phi(r) \varphi(R)$ and rewriting the variables on the RHS as $r_{1}=R-r / 2$ and $r_{2}=R+r / 2$, we reach

$$
\begin{align*}
i \hbar \frac{\partial}{\partial t} \phi(r, t) \varphi(R, t) & =i \hbar[\dot{\phi}(r, t) \varphi(R, t)+\phi(r, t) \dot{\varphi}(R, t)] \\
& =[-\underbrace{\frac{\hbar^{2}}{4 m}}_{=2 M} \frac{\partial^{2}}{\partial R^{2}}-\underbrace{\frac{\hbar^{2}}{m}}_{=2 \mu} \frac{\partial^{2}}{\partial r^{2}}+A e^{-\frac{r^{2}}{2 S^{2}}}] \phi(r, t) \varphi(R, t) \tag{20}
\end{align*}
$$

with total mass $M$ and reduced mass $\mu$. For the spatial derivatives we used the relation $\frac{\partial}{\partial r_{1}}=\underbrace{\frac{\partial R}{\partial r_{1}}}_{=1 / 2} \frac{\partial}{\partial R}+\underbrace{\frac{\partial r}{\partial r_{1}}}_{=-1} \frac{\partial}{\partial r}$, and $\frac{\partial}{\partial r_{2}}=\underbrace{\frac{\partial R}{\partial r_{2}}}_{=1 / 2} \frac{\partial}{\partial R}+\underbrace{\frac{\partial r}{\partial r_{2}}}_{=+1} \frac{\partial}{\partial r}$.

We can clearly see that if we fulfill two separate TDSEs for the relative and centre-ofmass motion:

$$
\begin{align*}
i \hbar \dot{\varphi}(R, t) & =-\frac{\hbar^{2}}{2 M} \frac{\partial^{2}}{\partial R^{2}} \varphi(R, t)  \tag{21}\\
i \hbar \dot{\phi}(r, t) & =\left[-\frac{\hbar^{2}}{2 \mu} \frac{\partial^{2}}{\partial r^{2}}+A e^{-\frac{r^{2}}{2 S^{2}}}\right] \phi(r, t), \tag{22}
\end{align*}
$$

the original equation is fulfilled. The TDSE for the centre of mass, Eq. (21), is just that of a free particle, so it will e.g. show the diffusion behavior that you know from the free Gaussian wavepacket.
(4b) Discuss which symmetry properties the relative wavefunction $\phi(r)$ must have for indistinguishable Bosons and Fermions. How does that differ from distinguishable particles? [2 points]
Solution: Clearly the requirement that $\psi\left(r_{1}, r_{2}\right)= \pm \psi\left(r_{2}, r_{1}\right)$ translates into $\phi(r)=$ $\pm \phi(-r)$, i.e. the relative wavefunction must be symmetric or anti-symmetric around the origin. This is because $R$ does not change when flipping the two locations.


Figure 1: Relative probability density, using the stronger potential with amplitude $A_{1}=3$ for (left) distinguishable particles, (mid) Bosons and (right) Fermions.
(4c) The code Assignment1_phy635_program_draft_v1.xmds is setup to model scattering of the two particles discussed above for potential with $A=A_{1}=3$ and $S=2$, initially treating the particles as (i) distinguishable with initial wavefunction $\phi(r, t=$ $0)=\mathcal{N} e^{-\frac{\left(r-r_{0}\right)^{2}}{2 \sigma^{2}}} e^{-i k r}$ (do not change parameters of that wavepacket). Edit the code such that it can also treat the particles as (ii) Bosons and (iii) Fermions. For each of (i)-(iii) run it for the parameters above, as well as $A=A_{2}=0.8$. Use the script Assignment1_plot_reldens_v1.m to plot the probability density of the relative coordinate $r$ for all six cases. [3 points]
Solution: To adapt the code for Bosons and Fermions, we just have to make sure that the initial wavefunction is properly symmetrised or anti-symmetrised. See Assignment1_phy635_solution_v1.xmds, line 51. The relative probability density for the original parameters $\left(A_{1}\right)$, the "strong repulsive potential", is shown in Fig. 1 (please fip axes labels $r \rightarrow t$ in all figures, these are accidentally swapped). Since the particles strongly repel, they never occupy the same spatial region. Hence densities for Bosons and Fermions are identical, and could be gotten from the distinguishable ones by symmetrising the density.
 fip sides with some finite probability. This is best seen for distinguishable particles. Since they thus CAN be found in the same spatial region, the densities for Fermions and Bosons differ. In particular the density on the centre line ( $r=0$, means particles on top of each other), we have zero for Fermions and nonzero for Bosons.
(4d) Discuss and compare your six different results from (b) in the context of the cartoon shown in the lecture on page 12 (above Eq. (1.33)) [3 points]
Solution: The results illustrates that quantum mechanics gets into trouble with the con-


Figure 2: Relative probability density, using the weaker potential with amplitude $A_{2}=0.8$ for (left) distinguishable particles, (mid) Bosons and (right) Fermions.
cept of indistinguishable particles (only if) these reach the same spatial region, and due to the uncertainty of the wavepacket we can no longer trace a particle. If they repel so strongly that they do NOT enter the same region, I could in principle trace the wavepacket, but in this case it also does not matter whether the wavefunction is being symmetrised.

