# Multiple Particles 

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## 1 Second Quantization

The example of the Klein Paradox (particle production for scattering off of a step potential) focuses our attention on the number of particles occupying various states (scattering states in that case). There is a way of formulating quantum mechanics in which the number of particles occupying a particular state is the main computational focus. We'll start off with a discrete system, like the harmonic oscillator or infinite square well, where we have a Hamiltonian $H(x)$ and a set of single-particle eigenstates $\left\{\psi_{j}(x)\right\}_{j=0}^{\infty}$ with energies $\left\{E_{j}\right\}_{j=0}^{\infty}$ such that $H(x) \psi_{j}(x)=E_{j} \psi_{j}(x)$. We assume that the single particle states are orthonormal,

$$
\begin{equation*}
\int_{-\infty}^{\infty} \psi_{j}^{*}(x) \psi_{k}(x) d x=\delta_{j k} \tag{1}
\end{equation*}
$$

and complete, so that any normalizable $\psi(x)$ can be developed from a sum of the form

$$
\begin{equation*}
\psi(x)=\sum_{j=0}^{\infty} a_{j} \psi_{j}(x), \tag{2}
\end{equation*}
$$

with related identity,

$$
\begin{equation*}
\sum_{j=0}^{\infty} \psi_{j}^{*}(x) \psi_{j}\left(x^{\prime}\right)=\delta\left(x-x^{\prime}\right) \tag{3}
\end{equation*}
$$

As a check of this expression, take a square-integrable "test function" $f(x)$. We will show that

$$
\begin{equation*}
\int_{-\infty}^{\infty}\left[f(x) \sum_{j=0}^{\infty} \psi_{j}^{*}(x) \psi_{j}\left(x^{\prime}\right)\right] d x=f\left(x^{\prime}\right) \tag{4}
\end{equation*}
$$

First note that since $f(x)$ is square integrable, we can find $\left\{a_{k}\right\}_{k=0}^{\infty}$ such that

$$
\begin{equation*}
f(x)=\sum_{k=0}^{\infty} a_{k} \psi_{k}(x) \tag{5}
\end{equation*}
$$

Using this relation on the left in (4), we get

$$
\begin{align*}
\int_{-\infty}^{\infty} \sum_{j, k=0}^{\infty} a_{k} \psi_{j}^{*}(x) \psi_{k}(x) \psi_{j}\left(x^{\prime}\right) d x & =\sum_{j, k=0}^{\infty}\left[a_{k} \int_{-\infty}^{\infty} \psi_{j}^{*}(x) \psi_{k}(x) d x\right] \psi_{j}\left(x^{\prime}\right)  \tag{6}\\
& =\sum_{k=0}^{\infty} a_{k} \psi_{k}\left(x^{\prime}\right)=f\left(x^{\prime}\right)
\end{align*}
$$

as desired.

### 1.1 A Few Particles

Suppose now that we have two particles, one in the $j^{\text {th }}$ state, with wave function $\psi_{j}\left(x_{1}\right)$, the other in the $k^{\text {th }}$ state (for $j \neq k$ ), with wave function $\psi_{k}\left(x_{2}\right)$. We'd like a wave function $\psi\left(x_{1}, x_{2}\right)$ that allows us to combine the two particles. Adding the Hamiltonians together, as we would do classically, define $H\left(x_{1}, x_{2}\right)=H\left(x_{1}\right)+H\left(x_{2}\right)$. The product, $\psi\left(x_{1}, x_{2}\right)=\psi_{j}\left(x_{1}\right) \psi_{k}\left(x_{2}\right)$, is an eigenfunction of $H\left(x_{1}, x_{2}\right)$ :
$H\left(x_{1}, x_{2}\right) \psi_{j}\left(x_{1}\right) \psi_{k}\left(x_{2}\right)=H\left(x_{1}\right) \psi_{j}\left(x_{1}\right) \psi_{k}\left(x_{2}\right)+\psi_{j}\left(x_{1}\right) H\left(x_{2}\right) \psi_{k}\left(x_{2}\right)=\left(E_{j}+E_{k}\right) \psi_{j}\left(x_{1}\right) \psi_{k}\left(x_{2}\right)$.
To add more particles, just expand the product. For two particles with coordinates $x_{1}$ and $x_{2}$ in the $j^{\text {th }}$ state, and one with coordinate $x_{3}$ in the $k^{\text {th }}$ state, the Hamiltonian is $H\left(x_{1}, x_{2}, x_{3}\right)=H\left(x_{1}\right)+H\left(x_{2}\right)+H\left(x_{3}\right)$, and $\psi\left(x_{1}, x_{2}, x_{3}\right)=\psi_{j}\left(x_{1}\right) \psi_{j}\left(x_{2}\right) \psi_{k}\left(x_{3}\right)$ has

$$
\begin{equation*}
H\left(x_{1}, x_{2}, x_{3}\right) \psi\left(x_{1}, x_{2}, x_{3}\right)=\left(2 E_{j}+E_{k}\right) \psi\left(x_{1}, x_{2}, x_{3}\right) . \tag{8}
\end{equation*}
$$

Unsurprisingly, the energy here is just the number of particles in each state times the energy of that state.

We can stick with three particles but distribute them differently among the available energy levels: $\phi\left(x_{1}, x_{2}, x_{3}\right)=\psi_{j}\left(x_{1}\right) \psi_{k}\left(x_{2}\right) \psi_{k}\left(x_{3}\right)$ has two particles in the $k^{\text {th }}$ state with one in the $j^{\text {th }}$ state. It is clear that $\psi\left(x_{1}, x_{2}, x_{3}\right)$ and $\phi\left(x_{1}, x_{2}, x_{3}\right)$ are both normalized, since the single particle states are:

$$
\begin{equation*}
\int \psi^{*}\left(x_{1}, x_{2}, x_{3}\right) \psi\left(x_{1}, x_{2}, x_{3}\right) d x_{1} d x_{2} d x_{3}=1=\int \phi^{*}\left(x_{1}, x_{2}, x_{3}\right) \phi\left(x_{1}, x_{2}, x_{3}\right) d x_{1} d x_{2} d x_{3} . \tag{9}
\end{equation*}
$$

How about the overlap of these two different distributions of particles? Let's compute:

$$
\begin{align*}
\int \psi^{*}\left(x_{1}, x_{2}, x_{3}\right) \phi\left(x_{1}, x_{2}, x_{3}\right) d x_{1} d x_{2} d x_{3} & =\int \psi_{j}^{*}\left(x_{1}\right) \psi_{j}^{*}\left(x_{2}\right) \psi_{k}^{*}\left(x_{3}\right) \psi_{j}\left(x_{1}\right) \psi_{k}\left(x_{2}\right) \psi_{k}\left(x_{3}\right) d x_{1} d x_{2} d x_{3} \\
& =\int \psi_{j}^{*}\left(x_{2}\right) \psi_{k}\left(x_{2}\right) d x_{2}=0 \tag{10}
\end{align*}
$$

which shows that configurations with different numbers of particle per single-energy eigenstate are orthogonal.

Keeping track of all of the particles via a spatial wave function can get tedious, as the above calculations suggest. A natural abstract ket to describe the physical state of these systems is $\left|N_{j} N_{k}\right\rangle$, where $N_{j}$ is the number of particles in the $j^{\text {th }}$ state, and $N_{k}$ the number in the $k^{\text {th. }}$. First note that $\left\langle N_{j} N_{k} \mid N_{j} N_{k}\right\rangle=1$, the states are normalized since the single-particle ones are. Now suppose you have the overlap of $\left|N_{j} N_{k}+1\right\rangle$ with $\left|N_{j}+1 N_{k}\right\rangle$, so that we have the same total number of particles, but there is a mis-match in the singleparticle states that are occupied. From the example in (10), it is clear there will always be a non-overlapping pair, so that $\left\langle N_{j} N_{k}+1 \mid N_{j}+1 N_{k}\right\rangle=0$. More general occupation mismatches yield the same result. For a state $\left|N_{j} N_{k}\right\rangle$ and another $\left|N_{j}^{\prime} N_{k}^{\prime}\right\rangle$,

$$
\begin{equation*}
\left\langle N_{j}^{\prime} N_{k}^{\prime} \mid N_{j} N_{k}\right\rangle=\delta_{N_{j} N_{j}^{\prime}} \delta_{N_{k} N_{k}^{\prime}} \text { with } N_{j}+N_{k}=N_{j}^{\prime}+N_{k}^{\prime} . \tag{11}
\end{equation*}
$$

The matrix elements of the Hamiltonian, computed in the position basis as above, are

$$
\begin{equation*}
\left\langle N_{j}^{\prime} N_{k}^{\prime}\right| \hat{H}\left|N_{j} N_{k}\right\rangle=\left(N_{j} E_{j}+N_{k} E_{k}\right) \delta_{N_{j} N_{j}^{\prime}} \delta_{N_{k} N_{k}^{\prime}}, \tag{12}
\end{equation*}
$$

where $\hat{H}$ is the Hamiltonian operator (not necessarily written in the position basis). The multi-particle states are eigenstates of the Hamiltonian operator,

$$
\begin{equation*}
\hat{H}\left|N_{j} N_{k}\right\rangle=\left(N_{j} E_{j}+N_{k} E_{k}\right)\left|N_{j} N_{k}\right\rangle ., \tag{13}
\end{equation*}
$$

with energies that are fixed by the single-particle system,

$$
\begin{equation*}
E_{j}=\int \psi_{j}^{*}(x) H(x) \psi_{j}(x) d x \tag{14}
\end{equation*}
$$

The goal is to write $\hat{H}$ in terms of some other, "natural," operators.
To that end, working by analogy with the structure of the raising and lowering operators of the harmonic oscillator, define the action of $\hat{a}_{j}^{\dagger}$ on $\left|N_{j} N_{k}\right\rangle$ by

$$
\begin{equation*}
\hat{a}_{j}^{\dagger}\left|N_{j} N_{k}\right\rangle=\sqrt{N_{j}+1}\left|N_{j}+1 N_{k}\right\rangle \tag{15}
\end{equation*}
$$

so that the operator $\hat{a}_{j}^{\dagger}$ adds a particle of energy $N_{j}$ to the system. There is no reason to define such an operator in the non-relativistic case, because the Schrödinger equation does not involve a changing number of particles. But again referring to the Klein Paradox, relativistic forms of quantum mechanics can "produce" particles even via single-particle interactions with a potential, and it is this type of behavior that motivates the notation.

Going along with the "raising" operator, define $\hat{a}_{j}$ by its action on $\left|N_{j} N_{k}\right\rangle$ :

$$
\begin{equation*}
\hat{a}_{j}\left|N_{j} N_{k}\right\rangle=\sqrt{N_{j}}\left|N_{j}-1 N_{k}\right\rangle . \tag{16}
\end{equation*}
$$

This operator "removes" a particle of energy $N_{j}$. The numbers out front are normalizations that are reminiscent of the oscillator's raising and lowering operators. If we "add" a particle of energy $E_{j}$ then remove it,

$$
\begin{equation*}
\hat{a}_{j} \hat{a}_{j}^{\dagger}\left|N_{j} N_{k}\right\rangle=\hat{a}_{j} \sqrt{N_{j}+1}\left|N_{j}+1 N_{k}\right\rangle=\left(N_{j}+1\right)\left|N_{j} N_{k}\right\rangle, \tag{17}
\end{equation*}
$$

and the state $\left|N_{j} N_{k}\right\rangle$ is an eigenstate of the $\hat{a}_{j} \hat{a}_{j}^{\dagger}$ operator, with eigenvalue $N_{j}+1$. Similarly, removing, then adding a particle gives

$$
\begin{equation*}
\hat{a}_{j}^{\dagger} \hat{a}_{j}\left|N_{j} N_{k}\right\rangle=\hat{a}_{j}^{\dagger} \sqrt{N_{j}}\left|N_{j}-1 N_{k}\right\rangle=N_{j}\left|N_{j} N_{k}\right\rangle . \tag{18}
\end{equation*}
$$

This one's even better - the eigenvalue here is the number of particles in the $j^{\text {th }}$ state. The operator $\hat{a}_{j}^{\dagger} \hat{a}_{j}$ is called the "number operator." Taken together (17) and (18) give

$$
\begin{equation*}
\hat{a}_{j} \hat{a}_{j}^{\dagger}-\hat{a}_{j}^{\dagger} \hat{a}_{j}=1, \tag{19}
\end{equation*}
$$

defining the commutation relation for the creation and annihilation operators: $\left[\hat{a}_{j}, \hat{a}_{j}^{\dagger}\right]=1$.
The operators that create and remove particles of energy $E_{k}$, the $\hat{a}_{k}^{\dagger}$ and $\hat{a}_{k}$, behave similarly,

$$
\begin{equation*}
\hat{a}_{k}^{\dagger}\left|N_{j} N_{k}\right\rangle=\sqrt{N_{k}+1}\left|N_{j} N_{k}+1\right\rangle \quad \hat{a}_{k}\left|N_{j} N_{k}\right\rangle=\sqrt{N_{k}}\left|N_{j} N_{k}\right\rangle \quad\left[\hat{a}_{k}, \hat{a}_{k}^{\dagger}\right]=1 . \tag{20}
\end{equation*}
$$

The $\hat{a}_{k}$ and $\hat{a}_{j}$ operators do not talk to one another, acting as they do on particles of different energy:

$$
\begin{equation*}
\left[\hat{a}_{j}, \hat{a}_{k}\right]=0=\left[\hat{a}_{j}^{\dagger}, \hat{a}_{k}\right]=\left[\hat{a}_{j}^{\dagger}, \hat{a}_{k}^{\dagger}\right]=\left[\hat{a}_{j}, \hat{a}_{k}^{\dagger}\right] . \tag{21}
\end{equation*}
$$

There is a state that has no particles in the $j^{\text {th }}$ and $k^{\text {th }}$ single-particle states, $|00\rangle$, the "vacuum" here. If we act on this state with either $\hat{a}_{j}$ or $\hat{a}_{k}$, we should get zero, just as the lowering operator of the harmonic oscillator, acting on the ground state, gives zero. Above, we have tacitly assumed that neither $N_{j}$ nor $N_{k}$ are zero, but for completeness, we now record

$$
\begin{equation*}
\hat{a}_{j}\left|0 N_{k}\right\rangle=0 \quad \hat{a}_{k}\left|N_{j} 0\right\rangle=0, \tag{22}
\end{equation*}
$$

removing a particle that doesn't exist produces nothing.
The Hamiltonian operator's action on $\left|N_{j} N_{k}\right\rangle$ can now be written in terms of the creation and annihilation operators,

$$
\begin{equation*}
\hat{H}\left|N_{j} N_{k}\right\rangle=\left(E_{j} \hat{a}_{j}^{\dagger} \hat{a}_{j}+E_{k} \hat{a}_{k}^{\dagger} \hat{a}_{k}\right)\left|N_{j} N_{k}\right\rangle, \tag{23}
\end{equation*}
$$

giving, in this basis,

$$
\begin{equation*}
\hat{H}=E_{j} \hat{a}_{j}^{\dagger} \hat{a}_{j}+E_{k} \hat{a}_{k}^{\dagger} \hat{a}_{k} . \tag{24}
\end{equation*}
$$

We have focused on two different (single-particle) energy levels to keep the notation simple, but it is clear that to include any of the single-particle states all we need are the
occupation numbers: $N_{0}$ (number of particles in the ground state of the original Hamiltonian) $N_{1}$ (number of particles in the first excited state), etc. Each single particle energy eigenstate has its own creation and destruction operators, $\hat{a}_{0}^{\dagger}, \hat{a}_{0}, \hat{a}_{1}^{\dagger}, \hat{a}_{1}$, etc. The generic state is then an infinite string $\left|N_{0} N_{1} N_{2} \ldots N_{\ell} \ldots\right\rangle$. The generalization of (24) is

$$
\begin{equation*}
\hat{H}=\sum_{j=0}^{\infty} E_{j} \hat{a}_{j}^{\dagger} \hat{a}_{j} \tag{25}
\end{equation*}
$$

The multi-particle state with nothing in it is denoted $|0\rangle$ and called the "vacuum." A state with one particle in the $j^{\text {th }}$ state can then be constructed using $\hat{a}_{j}^{\dagger}$ : $\hat{a}_{j}^{\dagger}|0\rangle$. To get a state with 2 particles in the $j^{\text {th }}$ state, we apply $1 / 2 \hat{a}_{j}^{\dagger}$ to $\hat{a}_{j}^{\dagger}|0\rangle$, and so on. To get a state with $N_{j}$ particles, each with energy $E_{j}$, take

$$
\begin{equation*}
\frac{1}{\sqrt{N_{j}!}}\left(\hat{a}_{j}^{\dagger}\right)^{N_{j}}|0\rangle \tag{26}
\end{equation*}
$$

and similarly to populate other single particle eigenstates.
The expression in (25) generalizes for other operators that act on single-particle states. Let's write (25) in terms of the matrix elements, in position basis:

$$
\begin{equation*}
H_{n m} \equiv \int \psi_{n}^{*}(x) H(x) \psi_{m}(x) d x=\delta_{n m} E_{n} \tag{27}
\end{equation*}
$$

then

$$
\begin{equation*}
\hat{H}=\sum_{n, m=0}^{\infty} H_{n m} \hat{a}_{n}^{\dagger} \hat{a}_{m} \tag{28}
\end{equation*}
$$

The same procedure can be used to express other operators as sums of $\hat{a}^{\dagger} \hat{a}$. For a generic single particle operator that depends on position, $Q(x)$, the corresponding operator that acts on $\left|N_{0} N_{1} N_{2} \ldots N_{\ell} \ldots\right\rangle$ is:

$$
\begin{equation*}
\hat{Q}=\sum_{n, m=0}^{\infty} Q_{n m} \hat{a}_{n}^{\dagger} \hat{a}_{m} \quad Q_{n m} \equiv \int \psi_{n}^{*}(x) Q(x) \psi_{m}(x) d x \tag{29}
\end{equation*}
$$

So far, we have used the non-interacting single particle states of the original Hamiltonian, $H(x)$, with its external potential that depends only on the particle position, $V(x)$. Now we want to allow interactions between particles, a potential $V\left(x_{1}, x_{2}\right)$, like, for example, the Coulomb potential. How do operators like this behave when acting on the occupation kets? Just as $\hat{H}$ in (25) is a sum of of the single-particle Hamiltonian applied to each coordinate, we can form an operator that sums $V\left(x_{1}, x_{2}\right)$ over all coordinate pairs, being careful not to double-count:

$$
\begin{equation*}
V=\sum_{i>j} V\left(x_{i}, x_{j}\right) \tag{30}
\end{equation*}
$$

and then the analogue of (29) is

$$
\begin{equation*}
\hat{V}=\frac{1}{2} \sum_{i, j, k, \ell=0}^{\infty} Q_{i j k \ell} \hat{a}_{i}^{\dagger} \hat{a}_{j}^{\dagger} \hat{a}_{\ell} \hat{a}_{k} \quad Q_{i j k \ell} \equiv \iint \psi_{i}^{*}(x) \psi_{j}^{*}(y) V(x, y) \psi_{k}(x) \psi_{\ell}(y) d x d y \tag{31}
\end{equation*}
$$

For a Hamiltonian of the form: $-\frac{\hbar^{2}}{2 m} \frac{d^{2}}{d x^{2}} \psi(x)+U(x)+V(x, y), H(x)$ covers the kinetic and $U(x)$ piece of the potential, with $V(x, y)$ the interaction term. The corresponding occupancy number operator is

$$
\begin{equation*}
\hat{H}=\sum_{n, m=0}^{\infty} H_{n m} \hat{a}_{n}^{\dagger} \hat{a}_{m}+\frac{1}{2} \sum_{i, j, k, \ell=0}^{\infty} Q_{i j k \ell} \hat{a}_{i}^{\dagger} \hat{a}_{j}^{\dagger} \hat{a}_{\ell} \hat{a}_{k} \tag{32}
\end{equation*}
$$

### 1.2 Wave function operators

We know that $\hat{a}_{i}^{\dagger} \hat{a}_{i}$ tells us the number of particles in the $i^{\text {th }}$ single particle state,

$$
\begin{equation*}
\hat{a}_{i}^{\dagger} \hat{a}_{i}\left|N_{0} N_{1} \ldots N_{i-1} N_{i} N_{i+1} \ldots\right\rangle=N_{i}\left|N_{0} N_{1} \ldots N_{i-1} N_{i} N_{i+1} \ldots\right\rangle \tag{33}
\end{equation*}
$$

Notice that the occupancy state is an eigenvector of the operator. To count the total number of particles, we sum up the individual occupancies,

$$
\begin{equation*}
\hat{N} \equiv \sum_{i=0}^{\infty} \hat{a}_{i}^{\dagger} \hat{a}_{i} \tag{34}
\end{equation*}
$$

and then

$$
\begin{equation*}
\hat{N}\left|N_{0} N_{1} \ldots\right\rangle=\left(\sum_{i=0}^{\infty} N_{i}\right)\left|N_{0} N_{1} \ldots\right\rangle . \tag{35}
\end{equation*}
$$

We can build up linear combinations of the creation and annihilation operators. Define the operators

$$
\begin{equation*}
\hat{\psi}(x)=\sum_{i=0}^{\infty} \psi_{i}(x) \hat{a}_{i} \quad \hat{\psi}^{\dagger}(x)=\sum_{i=0}^{\infty} \psi_{i}^{*}(x) \hat{a}_{i}^{\dagger} \tag{36}
\end{equation*}
$$

where the coordinate (and potentially spin) dependence in $\psi_{i}(x)$ represents parameters of the operators $\hat{\psi}(x)$ and $\hat{\psi}^{\dagger}(x)$. The operator $\hat{a}_{i}^{\dagger}$ creates a particle with wave function $\psi_{i}(x)$, or informally, $\psi_{i}(x)=\langle x| \hat{a}_{i}^{\dagger}|0\rangle$. Then the operator $\hat{\psi}^{\dagger}(y)$ creates a particle with wave function:

$$
\begin{equation*}
\langle x| \hat{\psi}^{\dagger}(y)|0\rangle=\sum_{i=0}^{\infty} \psi_{i}^{*}(y) \psi_{i}(x)=\delta(x-y) \tag{37}
\end{equation*}
$$

a particle localized at $y$ (using (3)). Similarly, the operator $\hat{\psi}(y)$ destroys a particle located at $y$.

To see that the operator $\hat{\psi}^{\dagger}$ generates one and only one particle, act on $\hat{\psi}^{\dagger}(x)|0\rangle$ with $\hat{N}:$

$$
\begin{equation*}
\hat{N} \hat{\psi}^{\dagger}(x)|0\rangle=\sum_{j=0}^{\infty} \hat{a}_{j}^{\dagger} \hat{a}_{j}\left(\sum_{i=0}^{\infty} \psi_{i}^{*}(x) \hat{a}_{i}^{\dagger}|0\rangle\right)=\sum_{j=0}^{\infty} \sum_{i=0}^{\infty} \psi_{i}^{*}(x) \hat{a}_{j}^{\dagger} \hat{a}_{j} \hat{a}_{i}^{\dagger}|0\rangle \tag{38}
\end{equation*}
$$

and $\hat{a}_{j} \hat{a}_{i}^{\dagger}-\hat{a}_{i}^{\dagger} \hat{a}_{j}=\delta_{i j}$, so that

$$
\begin{equation*}
\hat{N} \hat{\psi}^{\dagger}(x)|0\rangle=\sum_{j=0}^{\infty} \sum_{i=0}^{\infty} \psi_{i}^{*}(x) \hat{a}_{j}^{\dagger}\left(\delta_{i j}+\hat{a}_{i}^{\dagger} \hat{a}_{j}\right)|0\rangle=\sum_{j=0}^{\infty} \sum_{i=0}^{\infty} \psi_{i}^{*}(x) \delta_{i j} \hat{a}_{j}^{\dagger}|0\rangle=\hat{\psi}^{\dagger}(x)|0\rangle \tag{39}
\end{equation*}
$$

(using $\hat{a}_{j}|0\rangle=0$ ). The eigenvalue of the $\hat{N}$ operator, acting on $\hat{\psi}^{\dagger}(x)|0\rangle$, is $N=1$.
The commutator structure for these new operators is inherited from the structure of the creation and annihilation operators:

$$
\begin{equation*}
[\hat{\psi}(x), \hat{\psi}(y)]=0 \tag{40}
\end{equation*}
$$

since $\left[\hat{a}_{i}, \hat{a}_{j}\right]=0$, and similarly for $\left[\hat{\psi}^{\dagger}(x), \hat{\psi}^{\dagger}(y)\right]=0$. For the commutator of $\hat{\psi}^{\dagger}(x)$ with $\hat{\psi}(y)$,

$$
\begin{equation*}
\left[\hat{\psi}(x), \hat{\psi}^{\dagger}(y)\right]=\sum_{i, j} \psi_{i}(x) \psi_{j}^{*}(y)\left[\hat{a}_{i}, \hat{a}_{j}^{\dagger}\right]=\sum_{i, j} \psi_{i}(x) \psi_{j}^{*}(y) \delta_{i j}=\sum_{i} \psi_{i}^{*}(x) \psi_{i}(y)=\delta(x-y) \tag{41}
\end{equation*}
$$

from (3) again.
The relations in (36) can be inverted to express the operators $\hat{a}_{j}$ and $\hat{a}_{j}^{\dagger}$ in terms of $\hat{\psi}(x)$ and $\hat{\psi}^{\dagger}(x)$. From the definition of $\hat{\psi}(x)$, multiply both sides by $\psi_{j}^{*}(x)$ (the single-particle wavefunction) and integrate over all space,

$$
\begin{equation*}
\int \psi_{j}^{*}(x) \hat{\psi}(x) d x=\sum_{i=0}^{\infty}\left(\int \psi_{j}^{*}(x) \psi_{i}(x) d x\right) \hat{a}_{i}=\hat{a}_{j} \tag{42}
\end{equation*}
$$

and similarly,

$$
\begin{equation*}
\int \psi_{j}(x) \hat{\psi}^{\dagger}(x) d x=\sum_{i=0}^{\infty}\left(\int \psi_{i}^{*}(x) \psi_{j}(x) d x\right) \hat{a}_{i}^{\dagger}=\hat{a}_{j}^{\dagger} \tag{43}
\end{equation*}
$$

Going back to the generic operator $\hat{Q}$ from (29), collect terms into sums that become the operators $\hat{\psi}(x)$ and $\hat{\psi}^{\dagger}(x)$ :

$$
\begin{align*}
\hat{Q} & =\sum_{n} \sum_{m} \hat{a}_{n}^{\dagger} \int \psi_{n}^{*}(x) Q(x) \psi_{m}(x) d x \hat{a}_{m}=\int\left[\sum_{n} \hat{a}_{n}^{\dagger} \psi_{n}^{*}(x) Q(x) \sum_{m} \hat{a}_{m} \psi_{m}(x)\right] d x  \tag{44}\\
& =\int \hat{\psi}^{\dagger}(x) Q(x) \hat{\psi}(x) d x
\end{align*}
$$

Similarly, the two-body potential operator is

$$
\begin{equation*}
\hat{V}=\frac{1}{2} \iint \hat{\psi}^{\dagger}(x) \hat{\psi}^{\dagger}(y) V(x, y) \hat{\psi}(y) \hat{\psi}(x) d x d y \tag{45}
\end{equation*}
$$

and then the Hamiltonian operator from (32) can be written as

$$
\begin{equation*}
\hat{H}=\int \hat{\psi}^{\dagger}(x) H(x) \hat{\psi}(x) d x+\frac{1}{2} \iint \hat{\psi}^{\dagger}(x) \hat{\psi}^{\dagger}(y) V(x, y) \hat{\psi}(y) \hat{\psi}(x) d x d y \tag{46}
\end{equation*}
$$

To make a "generic" state, act on the vacuum $|0\rangle$ with the position creation operator $\hat{\psi}^{\dagger}(x)$ and weighted by $f(x)$, then sum over all positions:

$$
\begin{equation*}
\int f(x) \hat{\psi}^{\dagger}(x)|0\rangle d x \tag{47}
\end{equation*}
$$

The resulting state, a continuous superposition of $\hat{\psi}^{\dagger}(x)|0\rangle$, is an eigenstate of the Hamiltonian operator $\hat{H}$,

$$
\begin{equation*}
\hat{H} \int f(x) \hat{\psi}^{\dagger}(x)|0\rangle d x=E \int f(x) \hat{\psi}^{\dagger}(x)|0\rangle d x \text {. } \tag{48}
\end{equation*}
$$

Using $\hat{\psi}(x)|0\rangle=0$ (since the $\hat{\psi}(x)$ operator is made up entirely of $\hat{a}_{i}$ operators, each of which returns zero when acting on the vacuum) and the commutator $\left[\hat{\psi}(x), \hat{\psi}^{\dagger}(y)\right]=\delta(x-y)$ to expand the left-hand side gives

$$
\begin{equation*}
\iint H(y) f(x) \hat{\psi}^{\dagger}(y) \hat{\psi}(y) \hat{\psi}^{\dagger}(x)|0\rangle d x d y=\int H(x) f(x) \hat{\psi}^{\dagger}(x)|0\rangle d x \tag{49}
\end{equation*}
$$

so that we must have $H(x) f(x)=E f(x)$ from the right-hand sides of (48) and (49). The weighting function satisfies the single-particle Schrödinger equation. The term that acts on pairs of particles went away because of the double $\hat{\psi}(x) \hat{\psi}(y)$ acting on $\hat{\psi}^{\dagger}(x)|0\rangle$. Starting with a state that has two particles, and a weighting function $f\left(x_{1}, x_{2}\right)$,

$$
\begin{equation*}
\int f\left(x_{1}, x_{2}\right) \hat{\psi}^{\dagger}\left(x_{1}\right) \hat{\psi}^{\dagger}\left(x_{2}\right)|0\rangle d x_{1} d x_{2} \tag{50}
\end{equation*}
$$

acting with $\hat{H}$, and requiring that the resulting state is an eigenstate, gives

$$
\begin{equation*}
\left[H\left(x_{1}\right)+H\left(x_{2}\right)+V\left(x_{1}, x_{2}\right)\right] f\left(x_{1}, x_{2}\right)=E f\left(x_{1}, x_{2}\right), \tag{51}
\end{equation*}
$$

where $V\left(x_{1}, x_{2}\right)$ is the interaction potential energy. The process continues for more and more particles. The wave functions we are used to from "ordinary" quantum mechanics emerge when we constrain the quantum field to a particular number of particles.

Finally, let's turn the whole procedure around, and imagine we were handed (46) as a classical Hamiltonian governing the complex field $\hat{\psi}(x, t)$ with a Hamiltonian $H(x)=$ $-\frac{\hbar^{2}}{2 m} \frac{d^{2}}{d x^{2}}+V(x)$. The operator equation of motion is given by

$$
\begin{equation*}
i \hbar \frac{\partial \hat{\psi}}{\partial t}=-[\hat{H}, \hat{\psi}]=H(x) \hat{\psi}, \tag{52}
\end{equation*}
$$

which is just Schrödinger's equation.
If we include the additional term for two-body interactions, we have to evaluate the commutator

$$
\begin{align*}
& {\left[\hat{\psi}(z), \iint V(x, y) \hat{\psi}^{\dagger}(x) \hat{\psi}^{\dagger}(y) \hat{\psi}(x) \hat{\psi}(y) d x d y\right]} \\
& =\iint\left(\delta(x-z)+\hat{\psi}^{\dagger}(x) \hat{\psi}(z)\right) \hat{\psi}^{\dagger}(y) \hat{\psi}(x) \hat{\psi}(y) V(x, y) d x d y  \tag{53}\\
& -\iint \hat{\psi}^{\dagger}(x)\left(\hat{\psi}(z) \hat{\psi}^{\dagger}(y)-\delta(y-z)\right) \hat{\psi}(x) \hat{\psi}(y) V(x, y) d x d y \\
& =\int \hat{\psi}^{\dagger}(y) \hat{\psi}(y) \hat{\psi}(z)(V(z, y)+V(y, z)) d y
\end{align*}
$$

Now, the operator equation of motion for $\hat{\psi}$ is

$$
\begin{equation*}
i \hbar \frac{\partial \hat{\psi}}{\partial t}=H(x) \hat{\psi}(x)+\frac{1}{2}\left[\int \hat{\psi}^{\dagger}(y) \hat{\psi}(y)[V(z, y)+V(y, z)] d y\right] \hat{\psi}(z) . \tag{54}
\end{equation*}
$$

If we take the potential between two particles to be a contact interaction, $V(x, y)=$ $V_{0} \delta(x-y)$, then the equation in (54) becomes

$$
\begin{equation*}
i \hbar \frac{\partial \hat{\psi}}{\partial t}=H \hat{\psi}+V_{0} \hat{\psi}^{\dagger} \hat{\psi} \hat{\psi} \tag{55}
\end{equation*}
$$

which is known as the "nonlinear Schrödinger equation." Using the non-local electromagnetic and/or gravitational potential $V(x, y)=k /|x-y|$, produces the more complicated

$$
\begin{equation*}
i \hbar \frac{\partial \hat{\psi}}{\partial t}=H \hat{\psi}+\left[k \int \frac{\hat{\psi}^{\dagger}(y) \hat{\psi}(y)}{\sqrt{y-z}} d y\right] \hat{\psi}(z) \tag{56}
\end{equation*}
$$

Finally, putting these two pieces together, and moving to a three-dimensional classical field point of view, we have Schrödinger's equation (specializing to gravity):

$$
\begin{equation*}
i \hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t}=-\frac{\hbar^{2}}{2 m} \nabla^{2} \psi(\mathbf{r}, t)+V_{0}|\psi(\mathbf{r}, t)|^{2} \psi(\mathbf{r}, t)-\operatorname{Gmm} \psi(\mathbf{r}, t) \int \frac{\left|\psi\left(\mathbf{r}^{\prime}, t\right)\right|^{2}}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|} d \tau^{\prime} \tag{57}
\end{equation*}
$$

From the form of this equation, we see that it can also be written using the auxiliary variable $\phi$ (a gravitational potential of sorts), via

$$
\begin{align*}
i \hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} & =-\frac{\hbar^{2}}{2 m} \nabla^{2} \psi(\mathbf{r}, t)+V_{0}|\psi(\mathbf{r}, t)|^{2} \psi(\mathbf{r}, t)+m \phi(\mathbf{r}, t) \psi(\mathbf{r}, t)  \tag{58}\\
\nabla^{2} \phi(\mathbf{r}, t) & =4 \pi G m \psi^{*}(\mathbf{r}, t) \psi(\mathbf{r}, t)
\end{align*}
$$

the "Schrödinger-Newton" system.

