Nonrelativistic Interacting Particles, All of Different Species

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Abstract Article 20554 introduced a model of a single nonrelativistic quantum particle with zero spin. This article describes a generalization to N interacting particles, all of different species.

Contents

1 Introduction

This article defines a simple model of N nonrelativistic quantum particles, all of different **species**. Different species means different observables: the observables associated with one species are distinct from the observables associated with another. Particles of different species are usually called **distinguishable**.[1] I'll refer to the model as the N**-species model**, with the understanding that it has only one particle of each species.

The model will be presented in a way that helps clarify how it relates to quantum field theory (QFT). QFT assigns (sets of) observables to regions of spacetime, not to individual particles. Such observables are called **local observables**. This article introduces the N-species model with an emphasis on its *local* observables. The model has different local observables for different species, including observables that detect the presence/absence of a given species in a given region of space at a given time.[2] I'll call them **detection observables**.

The particles in this model all interact with each other, which makes this model significantly more interesting – and more challenging! – than the single-particle model that was described in article 20554. The particles in this model all have zero spin (no intrinsic angular momentum). Their masses may all be different,[3] but they're not required to be different. Even if their masses are all equal, the particles are still of different species, because they are still detected by different observables.

[1] In contrast, two particles of the same species share the same observables. They are usually called **identical** or **indistinguishable**. Simple models of indistinguishable particles will be described in separate articles.

[2] This article mostly uses the Heisenberg picture (article 22871).

[3] Specifying their masses is part of the task of specifying the model.

2 Notation

Throughout this article, D denotes the number of spatial dimensions, and boldface denotes a quantity with D components, as in $\mathbf{x} = (x_1, ..., x_D)$. The standard abbreviations

$$\mathbf{x}\cdot\mathbf{y} \equiv x_1 y_1 + \cdots + x_D y_D \qquad\qquad \mathbf{x}^2 \equiv x_1^2 + \cdots + x_D^2$$

will be used.

The Hilbert space will be described using functions of the form $\psi(\mathbf{x}_1, ..., \mathbf{x}_N)$. A subscript on a boldface quantity is a species index, so $\mathbf{x}_n$ is associated with the nth species. The quantity $\mathbf{x}_n$ has D components, one for each dimension of space, so we need a notation that distinguishes between the *species* index and the *spatial* index. For the rest of this article, the $d$the spatial component $\mathbf{x}_n$ will be denoted $(\mathbf{x}_n)_d$. This is a single real variable. Altogether, $\psi(\mathbf{x}_1, ..., \mathbf{x}_N)$ denotes a function of $N \times D$ real variables. In an expression like

$$\int \left|\psi(\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N)\right|^2,$$

the symbol $\int$ denotes the integral over all of these $N \times D$ variables.

The gradient with respect to $\mathbf{x}_n$ will be denoted ∇_n, and its dth component will be denoted $(\nabla_n)_d$. Explicitly:

$$(\nabla_n)_d \equiv \frac{\partial}{\partial(\mathbf{x}_n)_d}.$$

The dot product of $\mathbf{x}_j$ and $\mathbf{x}_k$ is

$$\mathbf{x}_j \cdot \mathbf{x}_k \equiv (\mathbf{x}_j)_1(\mathbf{x}_k)_1 + \cdots + (\mathbf{x}_j)_D(\mathbf{x}_k)_D.$$

This two-subscript notation is a little cumbersome, but we'll rarely need to write the spatial index explicitly. In most equations, only the species index will need to be written explicitly.

3 Preview

This section previews a few important properties of the model. The model will be constructed explicitly in sections 4-6.

For any region R of space and any time t, the model has projection operators $Q_1(R,t)$, ... $Q_N(R,t)$, one for each species.[4] The complementary projection operator $1 - Q_n(R,t)$ will be abbreviated $\overline{Q}_n(R,t)$. A detection observable for the nth species is represented by a pair $\{Q_n(R,t),\, \overline{Q}_n(R,t)\}$. These projection operators represent the two possible outcomes when the observable is measured: the outcome $Q_n(R,t)$ means that the one-and-only particle of the nth species is (at least momentarily) localized entirely inside R at time t, and the outcome $\overline{Q}_n(R,t)$ means it's localized entirely outside of R at time t.

The model has symmetry under translations in space and time: it has a continuous family of unitary operators $U(\mathbf{x},t)$ for which[5]

$$Q_n(R+\delta\mathbf{x}, t+\delta t) = U^{-1}(\delta\mathbf{x},\delta t)Q_n(R,t)U(\delta\mathbf{x},\delta t) \tag{1}$$

$$U(\mathbf{x}_1,t_1)U(\mathbf{x}_2,t_2) = U(\mathbf{x}_1+\mathbf{x}_2,\, t_1+t_2) \tag{2}$$

for all n. Equation (2) implies that all of these unitary operators commute with each other, so Stone's theorem says that they can all be written as

$$U(\mathbf{x},t) = \exp\left(\frac{-i}{\hbar}(\mathbf{x}\cdot\mathbf{P} + tH)\right) \tag{3}$$

for some fixed set of mutually commuting self-adjoint operators $P_1, ..., P_D$ (collectively denoted $\mathbf{P}$) and H. The operator H that generates time translations is called the **Hamiltonian** or **(total) energy operator** (article 22871), and the operators P_k that generate space translations are called the **(total) momentum operators**.[6]

[4] These projection operators will be constructed in section 6.

[5] $R + \delta\mathbf{x}$ denotes the region obtained by translating R by an amount $\mathbf{x}$. In other words, $R+\delta\mathbf{x}$ consists of the points obtained by adding $\delta\mathbf{x}$ to the coordinates of the points in R.

[6] The Hamiltonian and momentum operators will be constructed in sections 5 and 7, respectively.

4 The Hilbert space

An element of the Hilbert space $\mathcal{H}$ will be represented by a complex-valued function

$$\psi(\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N) \tag{4}$$

of $N \times D$ real variables. A function ψ is called **normalizable** if the quantity[7]

$$\int \left|\psi(\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N)\right|^2 \tag{5}$$

is well-defined (not infinite). Only normalizable functions are used to represent elements of $\mathcal{H}$. Any function for which (5) is zero is said to have **zero norm**.[8] If the difference between two functions has zero norm, then they both represent the same element of $\mathcal{H}$.

When thinking of the Hilbert space in abstract terms, we can use the symbol $|\psi\rangle$ to denote the element of $\mathcal{H}$ represented by the function $\psi(\mathbf{x})$. A Hilbert space is a vector space, so $|\psi\rangle$ can also be called a **vector**. The inner product of two vectors $|\phi\rangle$ and $|\psi\rangle$ is defined by

$$\langle\phi|\psi\rangle \equiv \int \phi^*(\mathbf{x}_1, ..., \mathbf{x}_N)\psi(\mathbf{x}_1, ..., \mathbf{x}_N). \tag{6}$$

Despite appearances, the Hilbert spaces defined above for different N are all isomorphic to each other (as abstract Hilbert spaces): they are different ways of expressing the one and only infinite-dimensional separable Hilbert space over the complex numbers (article 90771). This means that *we cannot determine that this is an N-particle model just by looking at the Hilbert space.* Different models are distinguished from each other by the pattern of their observables, not by how the Hilbert space is presented.

[7] As promised in section 2, the symbol $\int$ here denotes the integral over all space for each argument $\mathbf{x}_n$.

[8] The quantity (5) can be zero even if the function ψ is not zero everywhere. A function that is nonzero only at a finite number of isolated points is an example of a function with zero norm.

5 The Hamiltonian

The Hamiltonian for the N-species model is

$$H = T + V \tag{7}$$

with T and V defined by[9]

$$T\psi(\mathbf{x}_1, ..., \mathbf{x}_N) \equiv \sum_n \frac{-(\hbar\nabla_n)^2}{2m_n}\psi(\mathbf{x}_1, ..., \mathbf{x}_N) \tag{8}$$

$$V\psi(\mathbf{x}_1, ..., \mathbf{x}_N) \equiv \sum_{j<k} V_{jk}(\mathbf{x}_j - \mathbf{x}_k)\psi(\mathbf{x}_1, ..., \mathbf{x}_N). \tag{9}$$

The parameter m_n is the mass of one particle of the nth species, and the function V_{jk} defines the interaction between species j and k.

[9] I'm using the notation that was introduced in article 20554: for any linear operator A on the Hilbert space, "$A\psi$" is the name of a function that represents the vector $A|\psi\rangle$.

6 Detection observables

For a given region R of space, the detection observables previewed in section 3 are defined for $t = 0$ by

$$Q_n(R,0)\psi(\mathbf{x}_1,...,\mathbf{x}_N) \equiv \begin{cases} \psi(\mathbf{x}_1,...,\mathbf{x}_N) & \text{if } \mathbf{x}_n \in R \\ 0 & \text{otherwise.} \end{cases} \tag{10}$$

The detection observables for other values of t are then defined using equations (1) and (3). Explicitly,

$$Q_n(R,t) = U^{-1}(t)Q_n(R,0)U(t) \tag{11}$$

where $U(t) \equiv U(\mathbf{0},t)$ is the time translation operator

$$U(t) \equiv e^{-iHt/\hbar} \tag{12}$$

and H is the Hamiltonian that was defined in section 5.

The assertion that the observable $Q_n(R,t)$ detects *something* in the region R at time t is an important input to the model's definition, but the assertion that it detects an *individual particle* is not really needed, because that could be inferred by studying how the thing that $Q_n(R,t)$ detects behaves over time. The key to defining the model is simply to specify which operators represent observables localized in each region of space at each time.

The detection observables defined above are not the model's only local observables, but we can use them to systematically specify which other operators can represent localized observables, where they are localized, and when. This is the rule: for an observable A to qualify as being localized in region R at time t, it must satisfy

$$AQ_1(\overline{R},t)\cdots Q_N(\overline{R},t)|\psi\rangle \propto Q_1(\overline{R},t)\cdots Q_N(\overline{R},t)|\psi\rangle$$

for all $|\psi\rangle$, where $\overline{R}$ is the complement of R (the largest region that does not intersect R). This rule is consistent with the general principle that observables localized in non-intersecting regions of space at the same time should commute with each other (article 21916).

This completes the construction of the model.

7 Translation symmetry and momentum

The model has symmetry under translations in space and time. Time translation symmetry is manifest in the definitions (11)-(12). To confirm space translation symmetry, consider the unitary operators $U(\mathbf{x})$ defined by

$$U(\mathbf{y})\psi(\mathbf{x}_1, ..., \mathbf{x}_N) = \psi(\mathbf{x}_1 - \mathbf{y}, ..., \mathbf{x}_N - \mathbf{y}). \tag{13}$$

According to equations (8)-(11), these operators satisfy[10]

$$U^{-1}(\mathbf{x})HU(\mathbf{x}) = H \qquad\qquad U^{-1}(\mathbf{x})Q_n(R,t)U(\mathbf{x}) = Q_n(R+\mathbf{x},t), \tag{14}$$

so equations (1)-(2) are satisfied by the operators

$$U(\mathbf{x},t) \equiv U(\mathbf{x})U(t)$$

with $U(t)$ defined by (12). From equations (3) and (13), the total momentum operators P_k are given by

$$P_k\psi(\mathbf{x}_1, ..., \mathbf{x}_N) = -i\hbar\sum_n (\nabla_n)_k\psi(\mathbf{x}_1, ..., \mathbf{x}_N),$$

where k is the spatial index and n is the species index (section 2). The first of equations (14) implies $P_kH = HP_k$, which then implies

$$U^{-1}(t)P_kU(t) = P_k,$$

so the total momentum is conserved.

[10] This relies on the fact that the functions V_{jk} depend only on the differences $\mathbf{x}_j - \mathbf{x}_k$.

8 Rotation symmetry and angular momentum

Now suppose that the functions $V_{jk}(\mathbf{x}_j-\mathbf{x}_k)$ depend only on the distances $|\mathbf{x}_j-\mathbf{x}_k|$. Then the model also has symmetry under rotations in space. To confirm this, let Λ be a $D\times D$ rotation matrix so that $\mathbf{x}\mapsto\Lambda\mathbf{x}$ is a coordinate rotation about the origin, and consider the unitary operators $U(\Lambda)$ defined by

$$U(\Lambda)\psi(\mathbf{x}_1,...,\mathbf{x}_N)=\psi(\Lambda^{-1}\mathbf{x}_1,...,\Lambda^{-1}\mathbf{x}_N).$$

Then

$$U^{-1}(\Lambda)Q_n(R,t)U(\Lambda)=Q_n(\Lambda R,t) \tag{15}$$

where ΛR is the result of rotating R about the origin (which may or may not be contained within R). For $t=0$, the result (15) is clear from equation (10). For other times t, it follows from the fact that the Hamiltonian is invariant under rotations:[11]

$$U^{-1}(\Lambda)HU(\Lambda)=H.$$

This implies that the generators of rotations – the **(total) angular momentum** operators – are invariant under translations in time. In other words, (each component of) the total angular momentum is conserved.

[11] This relies on the fact that the functions V_{jk} depend only on the distances $|\mathbf{x}_j-\mathbf{x}_k|$.

9 Boost symmetry

The model also has symmetry under an overall velocity shift, called a **boost**. This section shows that the unitary operator $U(\mathbf{v})$ defined by

$$U(\mathbf{v})\psi(\mathbf{x}_1,...,\mathbf{x}_N) = \exp\left(\frac{i}{\hbar}\mathbf{v}\cdot\sum_n m_n\mathbf{x}_n\right)\psi(\mathbf{x}_1,...,\mathbf{x}_N) \tag{16}$$

implements a boost with velocity $\mathbf{v}$:

$$U^{-1}(\mathbf{v})Q_n(R,t)U(\mathbf{v}) = Q_n(R+\mathbf{v}t,\, t). \tag{17}$$

To derive (17), start by using the definition (16) to get

$$-i\hbar\nabla_n U(\mathbf{v})\psi(\mathbf{x}_1,...,\mathbf{x}_N) = U(\mathbf{v})\left(m_n\mathbf{v} - i\hbar\nabla_n\right)\psi(\mathbf{x}_1,...,\mathbf{x}_N). \tag{18}$$

This implies

$$P_k U(\mathbf{v})\psi(\mathbf{x}_1,...,\mathbf{x}_N) = U(\mathbf{v})(Mv_k + P_k)\psi(\mathbf{x}_1,...,\mathbf{x}_N)$$

with $M \equiv \sum_n m_n$, so the boost shifts the system's total momentum by $M\mathbf{v}$. With H and V defined as in section (5), equation (18) also implies

$$\begin{aligned} HU(\mathbf{v})\psi(\mathbf{x}_1,...,\mathbf{x}_N) &= U(\mathbf{v})\left(\sum_n \frac{(m_n\mathbf{v}-i\hbar\nabla_n)^2}{2m_n} + V\right)\psi(\mathbf{x}_1,...,\mathbf{x}_N) \\ &= U(\mathbf{v})\left(H + \mathbf{v}\cdot\mathbf{P} + \frac{M\mathbf{v}^2}{2}\right)\psi(\mathbf{x}_1,...,\mathbf{x}_N), \end{aligned} \tag{19}$$

which gives

$$U(\mathbf{0},t)U(\mathbf{v}) = \exp\big(-iM\mathbf{v}^2t/2\hbar\big)U(\mathbf{v})U(\mathbf{v}t,t),$$

where $U(\mathbf{x},t)$ are the space and time translation operators defined earlier. Combine this with the identity $U^{-1}(\mathbf{v})Q_n(R,0)U(\mathbf{v}) = Q_n(R,0)$ to get (17).

10 The spectrum condition

One of the general requirements of quantum field theory[12] is the **spectrum condition**, which says that the spectrum of the Hamiltonian should have a finite lower bound (article 21916). This section shows that the N-species model satisfies the spectrum condition in the most important case, namely three-dimensional space ($D = 3$) with interaction terms of the Coulomb form

$$V_{jk}(\mathbf{x}) \propto \frac{1}{|\mathbf{x}|} \tag{20}$$

with $|\mathbf{x}| \equiv \sqrt{\mathbf{x}^2}$.

Start by writing the Hamiltonian as

$$H = \sum_{j<k} H_{jk} \tag{21}$$

with

$$H_{jk}\psi(\mathbf{x}_1, ..., \mathbf{x}_N) \equiv \left(-\frac{(\hbar\nabla_j)^2}{2(N-1)m_j} - \frac{(\hbar\nabla_k)^2}{2(N-1)m_k} + V_{jk}(\mathbf{x}_j - \mathbf{x}_k) \right) \psi(\mathbf{x}_1, ..., \mathbf{x}_N).$$

Each H_{jk} is the Hamiltonian of a two-species model with single-particle masses $(N-1)m_j$ and $(N-1)m_k$. The lower bound of the spectrum of an operator A is the infimum[13] $\langle\psi|A|\psi\rangle/\langle\psi|\psi\rangle$ among all nonzero vectors $|\psi\rangle$, which I'll abbreviate as $\inf(A)$. Equation (21) implies the inequality[14]

$$\inf(H) \geq \sum_{j<k} \inf(H_{jk}).$$

[12] Article 15939 explains that the N-species model is one of the **superselection sectors** of a nonrelativistic quantum field theory.

[13] The **infimum** of a quantity is its greatest lower bound. The infimum may exist even if the *minimum* does not. Example: the infimum of the set of positive real numbers is zero, even though the set of positive real numbers does not have a minimum (no positive real number is smaller than all of the others).

[14] This is an inequality instead of an equality, because a vector $|\psi\rangle$ that minimizes the left-hand side might not minimize any of the terms on the right-hand side. The reason is similar when *minimum* is replaced by *infimum*.

This says that if each term H_{jk} satisfies the spectrum condition, then so does H. Article 89695 shows that H_{jk} can be written

$$H_{jk} = H_{jk,\text{com}} + H_{jk,\text{rel}} \tag{22}$$

where the **center of mass** term $H_{jk,\text{com}}$ is formally the Hamiltonian for a single free particle with mass $(N-1)(m_j+m_k)$, and where the **relative motion** term $H_{jk,\text{rel}}$ is formally the Hamiltonian for a single particle with mass $(N-1)m_jm_k/(m_j+m_k)$ under the influence of an **external potenital** $V_{jk}(\mathbf{x})$. Equation (22) implies

$$\inf(H_{jk}) \geq \inf(H_{jk,\text{com}}) + \inf(H_{jk,\text{rel}}).$$

The fact that the center-of-mass term satisfies the spectrum condition is clear (article 20554). When $D=3$ and with an interaction term of the Coulomb form (20), the fact that the relative-motion term satisfies the spectrum condition is well-known.[15] Altogether, this shows that the N-species model satisfies the spectrum condition when $D=3$ and with an interaction term of the Coulomb form (20).

[15] Lieb (1990) gives a concise proof in equations (3.1)-(3.4) on pages 11-12. A less concise proof, using explicit solutions of the Schrödinger equation, is reviewed in many introductions to quantum mechanics under headings like *ground state of a hydrogen-like atom*.

11 Ideal measurement of a detection observable

Let $|\psi\rangle$ be a state-vector representing whatever we know about how the physical system was prepared before the measurement, and use the abbreviation

$$\rho(\cdots) \equiv \frac{\langle\psi|\cdots|\psi\rangle}{\langle\psi|\psi\rangle}. \tag{23}$$

Starting with this state, consider a perfect measurement of the detection observable $\{Q_n(R,t), \overline{Q}_n(R,t)\}$ for the nth species. The general principles of quantum theory (article 03431) say that the quantity

$$p \equiv \rho\big(Q_n(R,t)\big) \tag{24}$$

is the probability that we should assign to the possible outcome $Q_n(R,t)$ of the measurement. In other words, this is the probability that the outcome of the measurement will be "the particle of species n is localized entirely within R." The probability of the opposite outcome, "the particle of species n is localized entirely outside of R," is

$$\rho\big(\overline{Q}_n(R,t)\big) = 1 - p.$$

If the state-vector $|\psi\rangle$ is represented by a function (4), then equations (10) and (11) give this expression for the probability (24):

$$p = \frac{\int_{\mathbf{x}_n\in R} \Big|\psi(\mathbf{x}_1,...,\mathbf{x}_N,t)\Big|^2}{\int \Big|\psi(\mathbf{x}_1,...,\mathbf{x}_N,t)\Big|^2} \tag{25}$$

where the subscript in the numerator indicates that the domain of integration for $\mathbf{x}_n$ is limited to R, and $\psi(\mathbf{x}_1,...,\mathbf{x}_N,t)$ is a function representing the state-vector $U(t)|\psi\rangle$.

12 The Schrödinger equation

Thanks to equation (25), we can analyze the particles' behavior by analyzing the time-dependence of the function

$$\psi(\mathbf{x}_1, ..., \mathbf{x}_N, t) \equiv U(t)\psi(\mathbf{x}_1, ..., \mathbf{x}_N). \tag{26}$$

This way of representing the model's time-dependence is called the **Schrödinger picture**. The first part of this article used the Heisenberg picture, but the rest of this article uses the Schrödinger picture. The differential version of equation (26) is

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{x}_1, ..., \mathbf{x}_N, t) = H\psi(\mathbf{x}_1, ..., \mathbf{x}_N, t).$$

More explicitly,

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{x}_1, ..., \mathbf{x}_N, t) = \left(\sum_{n=1}^{N}\frac{-(\hbar\nabla_n)^2}{2m_n} + \sum_{j<k} V_{jk}(\mathbf{x}_j - \mathbf{x}_k)\right)\psi(\mathbf{x}_1, ..., \mathbf{x}_N, t). \tag{27}$$

Equation (27) is one example of a **Schrödinger equation**. After solving equation (27) subject to the initial condition

$$\psi(\mathbf{x}_1, ..., \mathbf{x}_N, 0) = \psi(\mathbf{x}_1, ..., \mathbf{x}_N),$$

we can use equation (25) to read off the probability that a measurement of the observable $\{Q_n(R,t), \overline{Q}_n(R,t)\}$ would give the outcome $Q_n(R,t)$.

13 Widely separated particles

Using the Schrödinger picture, consider an initial state of the form

$$\psi(\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N, 0) = f_1(\mathbf{x}_1) f_2(\mathbf{x}_2) \cdots f_N(\mathbf{x}_N), \tag{28}$$

and suppose that the functions f_n have widely separated supports so that their product is practically zero whenever at least one of the distances $|\mathbf{x}_j - \mathbf{x}_k|$ is large. According to equations (10) and (25), this means that the particles are widely separated at $t = 0$. Suppose also that the functions $V_{jk}(\mathbf{x}_j - \mathbf{x}_k)$ approach zero sufficiently rapidly as $|\mathbf{x}_j - \mathbf{x}_k| \to \infty$ so that interactions are negligible when the particles are widely separated. Then the interaction terms are effectively zero when acting on such states, so the unitary time evolution operators effectively factorize:

$$e^{-iHt/\hbar} \approx e^{-iH_1 t/\hbar} e^{-iH_2 t/\hbar} \cdots e^{-iH_N t/\hbar} \qquad \text{(for widely separated particles)}$$

with[16]

$$H_n \equiv \frac{-(\hbar \nabla_n)^2}{2m_n}.$$

The operator H_n is the Hamiltonian for a single free particle of the nth species. As long as the particles remain widely separated, this gives

$$\psi(\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N, t) \approx f_1(\mathbf{x}_1, t) f_2(\mathbf{x}_2, t) \cdots f_N(\mathbf{x}_N, t) \tag{29}$$

with

$$f_n(\mathbf{x}_n, t) \equiv e^{-iH_n t/\hbar} f_n(\mathbf{x}_n).$$

This says that the particles behave like free particles, oblivious to each others' existence. This is no longer true when the particles are closer together – when configurations with small $|\mathbf{x}_j - \mathbf{x}_k|$ make a significant contribution to the norm of $\psi(\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N, t)$. The functions $f_n(\mathbf{x}, t)$ are often called **wavepackets**.[17]

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[16] This equation is an abbreviation for "applying the linear operator H_n to a vector $|\psi\rangle$ is the same as applying the differential operator $-\nabla_n^2/2m_n$ to a function that represents the vector $|\psi\rangle$."

[17] Any localized wavepacket must eventually disperse (spread out), as emphasized in article 20554.

14 The motion of well-localized particles

Now allow the particles to be closer together, so that the effect of the interaction V is not negligible, but assume that the state remains approximately factorizable into distinct wavepackets (equation (29)), and assume that the wavepackets remain well-enough localized so that the functions V_{jk} are approximately constant over the width of any one of them. These assumptions aren't always true (section 15), but when they are, we will see that a classical model like the one described in article 33629 can be a good approximation.

The analysis is based on equation (25). Conceptually, our assumption that each of the wavepackets remains well-localized means that we can choose the region R for each species in a time-dependent way so that the quantity (25) remains close to 1, so that the particle would almost certainly be found there if that detection observable were measured. We can track those regions implicitly by considering the quantities

$$\overline{\mathbf{x}}_n(t) \equiv \frac{\int \big|\psi(t)\big|^2 \mathbf{x}_n}{\int \big|\psi(t)\big|^2}, \tag{30}$$

using the abbreviation

$$\psi(t) \equiv \psi(\mathbf{x}_1, ..., \mathbf{x}_N, t). \tag{31}$$

Equation (29) implies

$$\overline{\mathbf{x}}_n(t) \approx \frac{\int d^D x \ \big|f_n(\mathbf{x}, t)\big|^2 \mathbf{x}}{\int d^D x \ \big|f_n(\mathbf{x}, t)\big|^2},$$

so $\overline{\mathbf{x}}_n(t)$ indicates the location of the nth wavepacket at time t, as long as it remains localized well enough for "the location" to be a meaningful concept.

To streamline the analysis, let $\mathbf{X}_n$ denote the list of D operators defined collectively by

$$\mathbf{X}_n\psi(t) = \mathbf{x}_n\psi(t),$$

again using the abbreviation (31). For each species n, the symbol $\mathbf{X}_n$ represents a list of D different operators, one for each dimension of space, just like each $\mathbf{x}_n$

represents a list of D real variables. Similarly, let $\mathbf{P}_n$ denote the list of D operators defined collectively by

$$\mathbf{P}_n\psi(t) = -i\hbar\nabla_n\psi(t).$$

The operators in $\mathbf{X}_n$ and $\mathbf{P}_n$ are all self-adjoint.[18] Using this notation, the Hamiltonian defined in section 5 can also be written

$$H = \sum_n \frac{\mathbf{P}_n^2}{2m_n} + V$$

and the quantities (30) can be written

$$\overline{\mathbf{x}}_n(t) = \frac{\langle\psi|U^{-1}(t)\mathbf{X}_n U(t)|\psi\rangle}{\langle\psi|\psi\rangle} \tag{32}$$

where $|\psi\rangle$ is the state at the initial time $t = 0$. The denominator is independent of t because $U^{-1}(t)U(t) = 1$. Use the identities

$$\frac{d}{dt}U(t) = \frac{-i}{\hbar}HU(t) \qquad\qquad [\mathbf{X}_n, H] = \frac{i\hbar}{m_n}\mathbf{P}_n$$

to get

$$\begin{aligned}\frac{d}{dt}\overline{\mathbf{x}}_n(t) &= \frac{-i}{\hbar}\,\frac{\langle\psi|U^{-1}(t)\,[\mathbf{X}_n, H]\,U(t)|\psi\rangle}{\langle\psi|\psi\rangle}\\ &= \frac{1}{m_n}\,\frac{\langle\psi|U^{-1}(t)\mathbf{P}_n U(t)|\psi\rangle}{\langle\psi|\psi\rangle},\end{aligned}$$

[18] More carefully: these operators are defined only in a dense subset of the Hilbert space. They are self-adjoint within that dense subset.

and then use the identity $[\mathbf{P}_n, H] = [\mathbf{P}_n, V]$ to get[19]

$$\begin{aligned}\left(\frac{d}{dt}\right)^2 \overline{\mathbf{x}}_n(t) &= \frac{1}{m_n}\,\frac{d}{dt}\,\frac{\langle\psi|U^{-1}(t)\mathbf{P}_n U(t)|\psi\rangle}{\langle\psi|\psi\rangle} \\ &= \frac{-i}{\hbar m_n}\,\frac{\langle\psi|U^{-1}(t)\,[\mathbf{P}_n, H]\,U(t)|\psi\rangle}{\langle\psi|\psi\rangle} \\ &= \frac{-i}{\hbar m_n}\,\frac{\langle\psi|U^{-1}(t)\,[\mathbf{P}_n, V]\,U(t)|\psi\rangle}{\langle\psi|\psi\rangle} \\ &= \frac{-1}{m_n}\sum_{k\neq n}\frac{\int \psi^*(t)\,\nabla_n V_{nk}(\mathbf{x}_n - \mathbf{x}_k)\,\psi(t)}{\langle\psi|\psi\rangle},\end{aligned}$$

using the abbreviation (31) again. If the wavepackets remain distinct and well-localized, then we can use the approximation

$$\frac{\int \psi^*(t)\,\nabla_n V_{nk}(\mathbf{x}_n - \mathbf{x}_k)\,\psi(t)}{\langle\psi|\psi\rangle} \approx \nabla_n V_{nk}\big(\overline{\mathbf{x}}_n - \overline{\mathbf{x}}_k\big)$$

to get the final result

$$m_n\ddot{\overline{\mathbf{x}}}_n \approx -\sum_{k\neq n}\nabla_n V_{nk}\big(\overline{\mathbf{x}}_n - \overline{\mathbf{x}}_k\big), \tag{33}$$

where each overhead dot denotes a time-derivative. Equation (33) says that if the wavepackets remain distinct and well-localized, then the particles' behavior can be described using a classical model like the one used in article 33629.

[19] This is a special case of **Ehrenfest's theorem**.

15 Interaction, delocalization, and entanglement

The previous section assumed that the state remains approximately factorizable into distinct wavepackets (equation (29)) and that the wavepackets remain relatively well localized. When those assumptions are true, classical physics can be a good approximation.

However, situations in which those assumptions hold are only a tiny subset of what can happen in the N-species model. **Scattering theory**[20] often deals with situations in which particles come so close together that the functions V_{jk} are not approximately constant over the widths of the wavepackets. In this case, the particles tend to become delocalized as a result of the interaction, even more so than they eventually would anyway because of dispersion (article 20554). Interactions also generally cause the particles to become **entangled** with each other, which simply means that the state can no longer be represented by a function with the factorized form (29), even if it could initially. The fact that interactions generally lead to entanglement is clear from the fact that almost all vectors in the Hilbert space represent entangled states.[21] Quantum physics is much richer than classical physics.

[20] The word *theory* here refers to a collection of applications and computational methods, not to a different type of model.

[21] This, in turn, should be clear from the definition of *entangled*. Most multivariable functions cannot be written as a product of functions of fewer variables.

16 References

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