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ABSTRACT

Quantum mechanics is often developed in the position representation, but this is not necessary, and one can perform calculations in a representation-independent fashion, even for wavefunctions. In this work, we illustrate how one can determine wavefunctions, aside from normalization, using only operators and how those operators act on state vectors. To do this in plane polar and spherical coordinates requires one to convert the translation operator into those coordinates. As examples of this approach, we illustrate the solution of the Coulomb problem in two and three dimensions without needing to express any operators in position space.

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I. INTRODUCTION

The quantum-mechanical position-space translation operator

$$\widehat{T}(\vec{r}) = e^{-\frac{i}{\hbar}\vec{r}\cdot\hat{\vec{p}}} = e^{-\frac{i}{\hbar}\left(r_x\hat{p}_x + r_y\hat{p}_y + r_z\hat{p}_z\right)} \tag{1}$$

is normally expressed in terms of Cartesian components,

$$\vec{r} = \vec{e}_x r_x + \vec{e}_y r_y + \vec{e}_z r_z, \ \hat{\vec{p}} = \vec{e}_x\hat{p}_x + \vec{e}_y\hat{p}_y + \vec{e}_z\hat{p}_z, \tag{2}$$

with $\vec{e}_x$, $\vec{e}_y$, and $\vec{e}_z$ being the Cartesian unit vectors. We use hats to denote the operators on the state vector space. Note, in particular, that the quantities r_α in the translation operator are dimensionful numbers, not operators. The position and momentum operators satisfy the canonical commutation relation

$$[\hat{r}_\alpha, \hat{p}_\beta] = i\hbar\delta_{\alpha,\beta}, \tag{3}$$

where α and β run over the Cartesian dimensions.

The translation operator can be employed to determine position eigenstates by translating the position-space eigenvector at the origin, $|0_{\vec{r}}\rangle$, which satisfies

$$\hat{r}_\alpha|0_{\vec{r}}\rangle = 0. \tag{4}$$

One of our assumptions is that such a position eigenvector at the origin *exists*, without worrying about the details of rigged Hilbert spaces; we will see that the wavefunction at any position can be determined relative to the wavefunction at the origin. We then have the position-operator

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eigenstates given by

$$|\vec{r}\rangle = \widehat{T}(\vec{r})\,|0_{\vec{r}}\rangle. \tag{5}$$

It is easy to verify that

$$\hat{r}_\alpha|\vec{r}\rangle = r_\alpha|\vec{r}\rangle \tag{6}$$

by using the braiding relation (derived from the Hadamard lemma)

$$e^{\hat{A}} f(\hat{B}) e^{-\hat{A}} = f\left(\hat{B} + [\hat{A},\hat{B}] + \frac{1}{2!}[\hat{A},[\hat{A},\hat{B}]] + \frac{1}{3!}[\hat{A},[\hat{A},[\hat{A},\hat{B}]]] + \cdots\right), \tag{7}$$

which is valid, provided that $f(\hat{B})$ can be written as a sum of non-negative integral powers of $\hat{B}$ and the argument of the function on the right-hand side is a sum of terms consisting of increasingly nested commutators. For the verification of the position eigenstate, one simply notes that the commutator of position with momentum is a dimensionful number, and so it commutes with all operators, which truncates the series after the first commutator.

In this work, we discuss how to calculate wavefunctions using a representation-independent approach. This sounds like a contradiction since a wavefunction is the representation of a quantum state vector in a particular basis. However, because each component of the wavefunction is constructed from the inner product between the state ket and a basis bra, one can see that each component is an inner product between two vectors in the state vector space and hence is a representation-independent object. The representation only enters when we compute the components for *all* basis vectors in the given representation and represent the quantum state as a linear superposition over the basis vectors of the representation. Since the wavefunction (or the set of components of the expansion) is constructed from the representation-independent inner products, it can be found in a representation-independent fashion, as will be illustrated below.

The strategy of the representation-independent approach to quantum mechanics is then to write the position-space wavefunction of a state $|\psi\rangle$ in terms of the position eigenstate at the origin and the translation operator according to

$$\psi(\vec{r}) = \langle\vec{r}|\psi\rangle = \langle 0_{\vec{r}}|\widehat{T}^{\,\dagger}(\vec{r})|\psi\rangle. \tag{8}$$

This expression provides a route to solely evaluate the wavefunction by manipulating operators. This is because when the position operator acts on the position eigenstate at the origin, it *annihilates* the state at the origin [see Eq. (4)]. To carry out these calculations for energy eigenfunctions, one needs to factorize the Hamiltonian, in order to determine what happens when the momentum operator acts on the state $|\psi\rangle$, using the methodology of the Schrödinger factorization method.[1–3]

We term this approach a representation-independent way to calculate the wavefunctions because one does not need to express the operators used to determine the state vectors in the specific basis of the wavefunctions. Instead, we only employ the commutation relations of the operators to determine the wavefunctions (up to overall normalization). For example, when working with the momentum operator, we only use the canonical commutation relation and how the momentum operator acts on the energy eigenstate. We do not need to use $\hat{\vec{p}} = -i\hbar\nabla$, the position-space representation of the momentum operator.

Böhm illustrated an alternate way to calculate wavefunctions in a representation-independent fashion,[4] and Merzbacher also used this approach.[5] Matrix elements of the position operator between energy eigenstates of the simple harmonic oscillator were employed to determine recurrence relations between energy eigenfunctions of different energy eigenvalues, but at the same position. The recurrence relations were then solved in terms of Hermite polynomials, eventually yielding the usual position-space wavefunctions. The general approach we develop here instead fixes the eigenfunction and relates the value of the wavefunction at the origin to the value of the wavefunction at $\vec{r}$. This latter approach can be generalized to many different problems other than the simple harmonic oscillator. It is not clear whether the method developed by Böhm can be extended beyond the simple harmonic oscillator. Moreover, our approach can also be employed for momentum-space wavefunctions.

We illustrate this process below. However, before doing so, we point out the reason why we need to transform the translation operator to spherical and plane polar coordinates. Spherically symmetric problems, such as the Coulomb problem, have wavefunctions that are explicit functions of

$$r = \sqrt{r_x^2 + r_y^2 + r_z^2}. \tag{9}$$

Such functions, for odd powers of r, cannot be expanded in a Maclauren series in the Cartesian position components because expansions about the origin in position space do not exist. Hence, one cannot use the Cartesian-basis representation of the translation operator. A similar argument applies for plane polar coordinates.

In Sec. II, we provide the details of how to convert the translation operator from the expression in terms of Cartesian components of the momentum operator to an expression in terms of the components of the momentum operator in spherical and plane polar coordinates. The exact operator expression can be simplified when it acts on $|0_{\vec{r}}\rangle$, which is the final form we employ to calculate wavefunctions. In Sec. III, we employ this approach to calculate the position-space wavefunctions for two- and three-dimensional Coulomb problems. This methodology is based on Schrödinger's factorization method. We conclude in Sec. IV. In the Appendix, we summarize technical details, primarily related to computing commutators in a representation-independent fashion.

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II. TRANSLATION OPERATOR IN SPHERICAL COORDINATES

To work with a three-dimensional spherically symmetric system, we express the translation operator, $\widehat{T}(\vec{r})$, in terms of the spherical coordinates, r, θ, and ϕ; the corresponding position operators, $\hat{r}$, $\cos\hat{\theta}$, $\sin\hat{\theta}$, $\cos\hat{\phi}$, $\sin\hat{\phi}$ and $\hat{p}_r$, $\hat{p}_\theta$, $\hat{p}_\phi$, the spherical components of the momentum operator, $\hat{\vec{p}}$. We use the spherical components of $\hat{\vec{p}}$, instead of the canonical momenta, because this is the cleanest way to decompose the inner product $\vec{r}\cdot\hat{\vec{p}}$. Note that $\hat{p}_r$ is a canonical momentum operator because it is the quantum analog of the classical momentum conjugate to the radial degree of freedom, whereas the same is not true for $\hat{p}_\theta$ and $\hat{p}_\phi$. We can still express the translation operator in terms of $\hat{p}_r$, $\hat{p}_\theta$, and $\hat{p}_\phi$ even though $\hat{p}_r$ is Hermitian, but not self-adjoint, and thus is not an observable. In addition, the translation operator remains unitary regardless of the coordinate system in terms of which it is expressed.

There is a subtle point associated with the symbol $|0_{\vec{r}}\rangle$: while $\vec{r}=0$ implies that $r_x=r_y=r_z=0$, it only implies that $r=0$ in spherical coordinates. That is, the values of θ and ϕ are indeterminate until specified by some limiting procedure for how the origin is approached. We will use what we call a "north-pole" state oriented along the positive z axis for definiteness.

It is well known that defining operators corresponding to the angles $\hat{\theta}$ and $\hat{\phi}$ is problematic.[6] Instead, we define the values corresponding to the position eigenstates expressed in spherical coordinates through the cosine or sine of those operators, which are always well defined in terms of $\hat{r}_\alpha$. In particular,

$$\cos\hat{\theta}=\frac{\hat{r}_z}{\hat{r}},\ \sin\hat{\theta}=\frac{\hat{\rho}}{\hat{r}},\ \cos\hat{\phi}=\frac{\hat{r}_x}{\hat{\rho}},\ \sin\hat{\phi}=\frac{\hat{r}_y}{\hat{\rho}}, \tag{10}$$

where

$$\hat{r}=\sqrt{\hat{r}_x^{\,2}+\hat{r}_y^{\,2}+\hat{r}_z^{\,2}}\ \text{ and }\ \hat{\rho}=\sqrt{\hat{r}_x^{\,2}+\hat{r}_y^{\,2}}. \tag{11}$$

These are all well-defined, but care must be taken when these operators act on position eigenstates that approach the origin.

Arguably, the easiest way to go from $|0_{\vec{r}}\rangle$ to $|\vec{r}\rangle$, using spherical coordinates, is to first translate a distance r in the z-direction, rotate by θ about the y axis, and then rotate by ϕ about the z axis, as illustrated in Fig. 1. Indeed, this is the common way to define the spherical coordinates r, θ, and ϕ. The operator needed to do this is

$$\widehat{T}(\vec{r})=e^{-\frac{i}{\hbar}\phi\hat{L}_z}e^{-\frac{i}{\hbar}\theta\hat{L}_y}e^{-\frac{i}{\hbar}r\hat{p}_z}e^{\frac{i}{\hbar}\theta\hat{L}_y}e^{\frac{i}{\hbar}\phi\hat{L}_z}, \tag{12}$$

and we discuss below the subtleties associated with how it operates on $|0_{\vec{r}}\rangle$. Here, $\hat{L}_y$ and $\hat{L}_z$ are the y- and z-components, respectively, of $\hat{\vec{L}}=\hat{\vec{r}}\times\hat{\vec{p}}$, the orbital angular momentum operator.

To establish this result, we use the braiding relation twice. First, we note that

$$e^{-\frac{i}{\hbar}\theta\hat{L}_y}e^{-\frac{i}{\hbar}r\hat{p}_z}e^{\frac{i}{\hbar}\theta\hat{L}_y}=e^{-\frac{i}{\hbar}r(\sin\theta\,\hat{p}_x+\cos\theta\,\hat{p}_z)} \tag{13}$$

and then

$$\begin{aligned}\widehat{T}(\vec{r})&=e^{-\frac{i}{\hbar}\phi\hat{L}_z}e^{-\frac{i}{\hbar}r(\sin\theta\hat{p}_x+\cos\theta\hat{p}_z)}e^{-\frac{i}{\hbar}\phi\hat{L}_z}\\&=e^{-\frac{i}{\hbar}r\left(\sin\theta\,\cos\phi\,\hat{p}_x+\sin\theta\,\sin\phi\,\hat{p}_y+\cos\theta\,\hat{p}_z\right)}.\end{aligned} \tag{14}$$

Since

$$r_x=r\,\sin\theta\,\cos\phi,\ \ r_y=r\,\sin\theta\,\sin\phi,\ \ \text{and}\ \ r_z=r\,\cos\theta, \tag{15}$$

Eq. (14) obviously yields the translation operator as expressed in Cartesian coordinates in Eq. (1).

We use Eqs. (A12) and (A13) to express $\hat{p}_z$ in terms of the spherical components of momentum according to

$$\hat{p}_z=\left(\hat{p}_r-i\frac{\hbar}{2\hat{r}}\right)\cos\hat{\theta}-\hat{p}_\theta\,\sin\hat{\theta}. \tag{16}$$

Note that the ordering is important in the second term because $\sin\hat{\theta}$ does not commute with $\hat{p}_\theta$, but there is no ordering ambiguity with the first term. Equations (12) and (16) allow us to eliminate the Cartesian components of momentum from the translation operator and obtain

$$\widehat{T}(\vec{r})=e^{-\frac{i}{\hbar}\phi\hat{L}_z}e^{-\frac{i}{\hbar}\theta\hat{L}_y}e^{-\frac{i}{\hbar}r\left[\left(\hat{p}_r-i\frac{\hbar}{2\hat{r}}\right)\cos\hat{\theta}-\hat{p}_\theta\,\sin\hat{\theta}\right]}e^{\frac{i}{\hbar}\theta\hat{L}_y}e^{\frac{i}{\hbar}\phi\hat{L}_z}. \tag{17}$$

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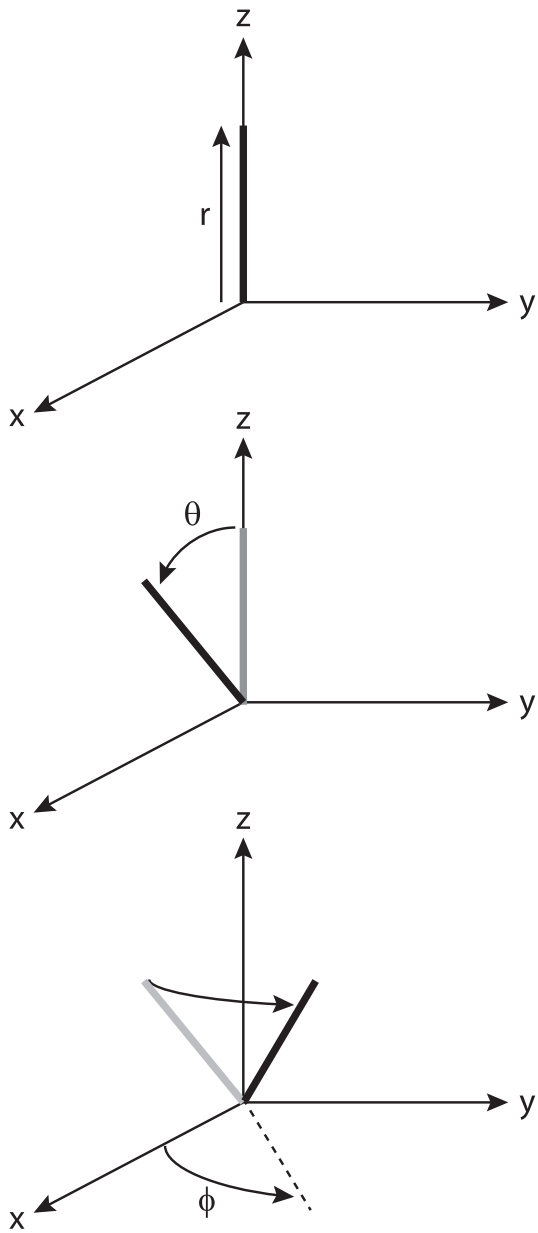

FIG. 1. Three-step process to move from the origin to (r_x, r_y, r_z): (top) first translate a distance r along the z axis, (middle) rotate about the y axis by an angle θ, and (bottom) rotate by an angle ϕ about the z axis. One can also reach the same point by rotating directly after the translation in the z-direction to the final point, or one can translate in the θ-direction in the $x - z$ plane and then rotate by ϕ, or one can translate in the θ, ϕ direction a distance r directly (not shown). All these alternatives lead to the same final point in space. The operators corresponding to each of these different ways to translate and rotate from the origin to the final point are shown in the main text.

We use Eq. (A13) and

$$\hat{\vec{e}}_\phi = -\vec{e}_x \sin\hat{\phi} + \vec{e}_y \cos\hat{\phi} \tag{18}$$

to re-express $\hat{p}_\theta$ according to

$$\hat{p}_\theta = \frac{1}{\hat{r}}\left(\hat{\vec{L}} \cdot \hat{\vec{e}}_\phi + i\frac{\hbar}{2}\cot\hat{\theta}\right) \tag{19}$$

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and thus transform the translation operator into its final form

$$\widehat{T}(\vec{r}) = e^{-\frac{i}{\hbar}\phi\hat{L}_z} e^{-\frac{i}{\hbar}\theta\hat{L}_y} e^{-\frac{i}{\hbar}r\left[\left(\hat{p}_r - i\frac{\hbar}{\hat{r}}\right)\cos\hat{\theta} - \frac{\hat{\vec{L}}\cdot\hat{\vec{e}}_\phi}{\hat{r}}\sin\hat{\theta}\right]} e^{\frac{i}{\hbar}\theta\hat{L}_y} e^{\frac{i}{\hbar}\phi\hat{L}_z}. \tag{20}$$

We emphasize that this is an operator equality. It is the expression of the translation operator in terms of spherical coordinates.

This operator relation can be rewritten in three other forms, which illustrate the different ways that one can derive the translation operator in spherical coordinates. First, note that $\hat{L}_z$ commutes with $\hat{r}$, $\cos\hat{\theta}$, $\sin\hat{\theta}$, $\hat{\vec{L}}\cdot\hat{\vec{e}}_\phi$, and $\hat{p}_r$ (or, more simply, it commutes with $\hat{p}_z$). This means that we can introduce the factor $\exp\left(\frac{i}{\hbar}\phi\hat{L}_z\right)\exp\left(-\frac{i}{\hbar}\phi\hat{L}_z\right)$ just to the left of the $\exp\left(\frac{i}{\hbar}\theta\hat{L}_y\right)$ term in Eq. (20) and then move the factor $\exp\left(\frac{i}{\hbar}\phi\hat{L}_z\right)$ to the left through the middle exponential factor, yielding

$$\widehat{T}(\vec{r}) = e^{-\frac{i}{\hbar}\phi\hat{L}_z} e^{-\frac{i}{\hbar}\theta\hat{L}_y} e^{\frac{i}{\hbar}\phi\hat{L}_z} e^{-\frac{i}{\hbar}r\left[\left(\hat{p}_r - i\frac{\hbar}{\hat{r}}\right)\cos\hat{\theta} - \frac{\hat{\vec{L}}\cdot\hat{\vec{e}}_\phi}{\hat{r}}\sin\hat{\theta}\right]} e^{-\frac{i}{\hbar}\phi\hat{L}_z} e^{\frac{i}{\hbar}\theta\hat{L}_y} e^{\frac{i}{\hbar}\phi\hat{L}_z}. \tag{21}$$

This form of the translation operator expresses it as a similarity transformation of the middle exponential factor with respect to the operator

$$e^{-\frac{i}{\hbar}\phi\hat{L}_z} e^{-\frac{i}{\hbar}\theta\hat{L}_y} e^{\frac{i}{\hbar}\phi\hat{L}_z} = e^{-\frac{i}{\hbar}\theta(-\hat{L}_x\,\sin\phi + \hat{L}_y\,\cos\phi)} \tag{22}$$

$$= e^{-\frac{i}{\hbar}\theta\vec{e}_\phi\,\cdot\,\hat{\vec{L}}}, \tag{23}$$

which follows from the braiding relation. Note that

$$\vec{e}_\phi\,\cdot\,\hat{\vec{L}} = -\hat{L}_x\,\sin\phi + \hat{L}_y\,\cos\phi \tag{24}$$

is a linear combination of the angular momentum operators with numbers, not operators, as coefficients because $\vec{e}_\phi$ is *not* an operator here. The translation operator then becomes

$$\widehat{T}(\vec{r}) = e^{-\frac{i}{\hbar}\theta\vec{e}_\phi\,\cdot\,\hat{\vec{L}}} e^{-\frac{i}{\hbar}r\left[\left(\hat{p}_r - i\frac{\hbar}{\hat{r}}\right)\cos\hat{\theta} - \frac{\hat{\vec{L}}\cdot\hat{\vec{e}}_\phi}{\hat{r}}\sin\hat{\theta}\right]} e^{\frac{i}{\hbar}\theta\vec{e}_\phi\,\cdot\,\hat{\vec{L}}}. \tag{25}$$

In this form of the translation operator, we first translate along the z axis a distance r and then rotate by an angle θ about an axis along $\vec{e}_\phi$, i.e., an axis rotated an angle ϕ counterclockwise from the y axis.

The final two ways we express the operator comes from a simple brute-force substitution. We solve Eqs. (A12)–(A.14) for $\hat{p}_x$, $\hat{p}_y$, and $\hat{p}_z$ in terms of $\hat{p}_r$, $\hat{p}_\theta$, and $\hat{p}_\phi$ and substitute into Eq. (1). Then, we use the inverse of the braiding relation to remove $\exp\left(-\frac{i}{\hbar}\theta\hat{L}_z\right)$ to the left and its Hermitian conjugate to the right. We also obtain this form by using the braiding relation to move the $\exp\left(-\frac{i}{\hbar}\theta\hat{L}_y\right)$ factor (and its conjugate) into the exponent in Eq. (20). This yields

$$\begin{aligned}\widehat{T}(\vec{r}) = e^{-\frac{i}{\hbar}\phi\hat{L}_z}\,\exp\Bigg(-\frac{i}{\hbar}r\Bigg\{&\left(\hat{p}_r - i\frac{\hbar}{\hat{r}}\right)\cos(\hat{\theta}-\theta) \\ &- \frac{1}{\hat{r}}\hat{\vec{L}}\cdot\hat{\vec{e}}_\phi\,\sin(\hat{\theta}-\theta) + \Bigg[\left(\hat{p}_r - i\frac{\hbar}{\hat{r}}\right)\sin\theta\,\sin\hat{\theta} \\ &+ \frac{1}{\hat{r}}\hat{\vec{L}}\cdot\hat{\vec{e}}_\phi\,\sin\theta\,\cos\hat{\theta}\Bigg](\cos\hat{\phi}-1) - \frac{\hat{L}_z}{\hat{r}}\frac{\sin\theta\,\sin\hat{\phi}}{\sin\hat{\theta}}\Bigg\}\Bigg)e^{\frac{i}{\hbar}\phi\hat{L}_z}.\end{aligned} \tag{26}$$

One can interpret this as a translation along the θ direction in the $x-z$ plane, followed by a rotation by ϕ about the z axis. If we use the braiding operation to move the remaining exponential factor into the exponent, we would have a single translation of length r along the θ, ϕ direction. We do not write that other final form explicitly here; it is given by the result in Eq. (26) without the exponential factors on the left and the right and with the substitution $\hat{\phi} \to \hat{\phi} - \phi$.

As one can immediately see, these forms for the translation operator are equivalent and are easily related by employing the braiding relation in different ways. They also have different physical interpretations for how the translation is performed. Of course, the operators in all four cases are identical and are just expressed in terms of different exponential factors.

The remaining task is to determine the proper limiting procedure to apply this operator on the position eigenstate at the origin. We derive it explicitly for the form of the translation operator given in Eq. (20), but the generalization for any of the other forms is straightforward to work out. Our final result is independent of which form is used.

The strategy is to perform a translation along $\vec{r}$ so that the indeterminate operators corresponding to $\cos\hat{\theta}$ and $\sin\hat{\theta}$ [when acting on $|0_{\vec{r}}\rangle$] can be properly defined. (It turns out that the indeterminacy with respect to ϕ need not be resolved in order to determine the final formula for the translation operator.) To this end, we introduce $\exp\left(\frac{i}{\hbar}\vec{\delta}\,\cdot\,\hat{\vec{p}}\right)\exp\left(-\frac{i}{\hbar}\vec{\delta}\,\cdot\,\hat{\vec{p}}\right) = 1$ to the left of $\widehat{T}(\vec{r})$. The vector $\vec{\delta}$ is an ordinary displacement vector, not an operator, and we choose it to be in the same direction as the vector $\vec{r}$ in the translation operator. We then move

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the rightmost exponential factor through $\widehat{T}(\vec{r})$ to the right, which we can do since it commutes with $\widehat{T}(\vec{r})$, as is easy to see when $\widehat{T}(\vec{r})$ is expressed in its Cartesian form in Eq. (1). We then operate on $|0_{\vec{r}}\rangle$, which yields

$$|\vec{r}\rangle = e^{\frac{i}{\hbar}\vec{\delta}\cdot\hat{\vec{p}}}\widehat{T}(\vec{r})e^{-\frac{i}{\hbar}\vec{\delta}\cdot\hat{\vec{p}}}|0_{\vec{r}}\rangle. \tag{27}$$

This equation can be re-expressed as

$$|\vec{r}\rangle = e^{\frac{i}{\hbar}\vec{\delta}\cdot\hat{\vec{p}}}\widehat{T}(\vec{r})|\delta_x,\delta_y,\delta_z\rangle. \tag{28}$$

Since the two rotation operators on the right-hand side of Eq. (20) first rotate by an angle $-\phi$ about the z axis and then by an angle $-\theta$ about the y axis, we find that the final position eigenstate, after the two rotations, points along the $+z$ axis. In other words, the choice that $\vec{\delta}$ lies in the same direction as $\vec{r}$ implies that

$$\tan\,\phi = \frac{\delta_y}{\delta_x} \tag{29}$$

so that

$$e^{\frac{i}{\hbar}\phi\hat{L}_z}|\delta_x,\delta_y,\delta_z\rangle = |\sqrt{\delta_x^2+\delta_y^2},0,\delta_z\rangle \tag{30}$$

and further implies that

$$\tan\,\theta = \frac{\sqrt{\delta_x^2+\delta_y^2}}{\delta_z} \tag{31}$$

so that

$$e^{\frac{i}{\hbar}\theta\hat{L}_y}e^{\frac{i}{\hbar}\phi\hat{L}_z}|\delta_x,\delta_y,\delta_z\rangle = |0,0,\delta\rangle. \tag{32}$$

Here,

$$\delta = \sqrt{\delta_x^2+\delta_y^2+\delta_z^2}. \tag{33}$$

Note that the ket $|0,0,\delta\rangle$ satisfies

$$\cos\hat{\theta}|0,0,\delta\rangle = \frac{\hat{r}_z}{\hat{r}}|0,0,\delta\rangle = |0,0,\delta\rangle \tag{34}$$

and

$$\sin\hat{\theta}|0,0,\delta\rangle = \frac{\hat{\rho}}{\hat{r}}|0,0,\delta\rangle = 0. \tag{35}$$

Because this is a state oriented along the north pole, the action of $\cos\hat{\phi}$ or $\sin\hat{\phi}$ on this ket is indeterminate, in the sense that one cannot determine the action of $\cos\hat{\phi}$ or $\sin\hat{\phi}$ on this state. Our goal is to simplify the form of the translation operator when it acts on this "north-pole" state. We expand the exponential function $\exp\left\{-\frac{i}{\hbar}\left[\left(\hat{p}_r - i\frac{\hbar}{\hat{r}}\right)\cos\hat{\theta} - \frac{\hat{\vec{L}}\cdot\hat{\vec{e}}_\phi}{\hat{r}}\sin\hat{\theta}\right]\right\}$ in a power series and use the action of $\cos\hat{\theta}$ and $\sin\hat{\theta}$ on the "north-pole" state [in Eqs. (34) and (35)]. Term by term in the power series expansion, we see that the exponential function simplifies and can be resummed to the form $\exp\left[-\frac{i}{\hbar}\left(\hat{p}_r - i\frac{\hbar}{\hat{r}}\right)\right]$ acting on the "north-pole" state. This produces

$$|\vec{r}\rangle = e^{\frac{i}{\hbar}\vec{\delta}\cdot\hat{\vec{p}}}e^{-\frac{i}{\hbar}\phi\hat{L}_z}e^{-\frac{i}{\hbar}\theta\hat{L}_y}e^{-\frac{i}{\hbar}r\left(\hat{p}_r - i\frac{\hbar}{\hat{r}}\right)}|0,0,\delta\rangle. \tag{36}$$

At this point, because $\hat{\vec{L}}$ commutes with $\hat{r}$ and $\hat{p}_r$, we can separate the radial and angular degrees of freedom according to

$$|\delta_x,\delta_y,\delta_z\rangle = e^{-\frac{i}{\hbar}\phi\hat{L}_z}e^{-\frac{i}{\hbar}\theta\hat{L}_y}|0,0,\delta\rangle = |r=\delta\rangle\otimes|\theta,\phi\rangle. \tag{37}$$

This result for the label of the state with $r=\delta$ arises because we define the radial coordinate eigenstates, $|r\rangle$, to satisfy

$$\hat{r}|r\rangle = r|r\rangle, \tag{38}$$

with r given by Eq. (9). One can immediately verify that $\hat{r}|\delta_x,\delta_y,\delta_z\rangle = \delta|\delta_x,\delta_y,\delta_z\rangle$, which establishes the use of the label $r=\delta$ in Eq. (37).

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We similarly define the angular state, $|\theta,\phi\rangle$, to be the state that satisfies

$$\cos\hat{\theta}|\theta,\phi\rangle = \cos\theta|\theta,\phi\rangle, \sin\hat{\theta}|\theta,\phi\rangle = \sin\theta|\theta,\phi\rangle, \tag{39}$$

$$\cos\hat{\phi}|\theta,\phi\rangle = \cos\phi|\theta,\phi\rangle, \sin\hat{\phi}|\theta,\phi\rangle = \sin\phi|\theta,\phi\rangle, \tag{40}$$

with one exception. The eigenvalue–eigenvector relations in Eq. (40) cannot be satisfied when the eigenvalues in Eq. (39) correspond to the cases where $\theta = 0$ or $\theta = \pi$.

Note that the operators $\hat{r}_x$, $\hat{r}_y$, and $\hat{r}_z$ cannot operate solely on the state $|r\rangle$, i.e., the domain of those operators lies outside of the space of the eigenstates of the radial-position operator $\hat{r}$. Similarly, they cannot act on the state $|\theta,\phi\rangle$. Of course, they can act on the tensor-product state $|r\rangle \otimes |\theta,\phi\rangle$.

However, we can allow the operator $\hat{r}$ to act only on $|r\rangle$ (and as the identity operator on $|\theta,\phi\rangle$) and $\cos\hat{\theta}$ (and the other similar trigonometric operators) act only on $|\theta,\phi\rangle$ (and as the identity on $|r\rangle$), as will be seen next. Consider $\cos\hat{\theta}$ acting on the state $|r\sin\theta\cos\phi, r\sin\theta\sin\phi, r\cos\theta\rangle = |r\rangle \otimes |\theta,\phi\rangle$, which is given by

$$\begin{aligned}
\cos\hat{\theta}|r\rangle \otimes |\theta,\phi\rangle &= \frac{\hat{r}_z}{\hat{r}}|r\rangle \otimes |\theta,\phi\rangle \\
&= e^{-\frac{i}{\hbar}\phi\hat{L}_z}\hat{r}_z e^{-\frac{i}{\hbar}\theta\hat{L}_y}\frac{1}{\hat{r}}|0,0,r\rangle \\
&= e^{-\frac{i}{\hbar}\phi\hat{L}_z}e^{-\frac{i}{\hbar}\theta\hat{L}_y}\underbrace{e^{\frac{i}{\hbar}\theta\hat{L}_y}\hat{r}_z e^{-\frac{i}{\hbar}\theta\hat{L}_y}}_{\text{braiding}}\frac{1}{\hat{r}}|0,0,r\rangle \\
&= e^{-\frac{i}{\hbar}\phi\hat{L}_z}e^{-\frac{i}{\hbar}\theta\hat{L}_y}\frac{-\sin\theta\hat{r}_x + \cos\theta\hat{r}_z}{\hat{r}}|0,0,r\rangle \\
&= \cos\theta|r\rangle \otimes |\theta,\phi\rangle.
\end{aligned} \tag{41}$$

We can accomplish this because the eigenvalue–eigenvector relationship given above is unchanged when we change the value of r in the radial ket. Hence, the operator $\cos\hat{\theta}$ acts as the identity on the $|r\rangle$ ket and can be taken to act solely on the $|\theta,\phi\rangle$ ket, yielding $\cos\hat{\theta}|\theta,\phi\rangle = \cos\theta|\theta,\phi\rangle$. We can proceed similarly to verify that this separation holds true for the three other trigonometric operators. The argument for the radial operator acting only on $|r\rangle$ can also be easily verified.

We can then take the limit $\delta \to 0^+$ so that $\exp\left(\frac{i}{\hbar}\vec{\delta}\cdot\hat{\vec{p}}\right) \to 1$. Gathering the final results together, we have established that

$$|\vec{r}\rangle = e^{-\frac{i}{\hbar}r\left(\hat{p}_r - i\frac{\hbar}{r}\right)}|r=0\rangle \otimes |\theta,\phi\rangle \tag{42}$$

and

$$\langle\vec{r}| = \langle\theta,\phi| \otimes \langle r=0|e^{\frac{i}{\hbar}r\left(\hat{p}_r + i\frac{\hbar}{r}\right)}. \tag{43}$$

These final expressions are a simplification of the translation operator in spherical coordinates when it acts on the state at the origin.

In order to calculate an energy wavefunction in position space, we must also decompose the energy eigenstate vector of the Hamiltonian according to a radial and angular momentum tensor-product state via

$$|\Psi\rangle = |\psi_r\rangle \otimes |l,m\rangle, \tag{44}$$

where the eigenvalues of $\hat{\vec{L}}^2$ and $\hat{L}_z$ (when acting on the state $|l,m\rangle$) are $l(l+1)\hbar^2$ and $m\hbar$, respectively. It follows that we can write the wavefunction as the product of the radial wavefunction and the angular momentum eigenfunction according to

$$\langle\vec{r}|\Psi\rangle = \langle r|\psi_r\rangle\langle\theta,\phi|l,m\rangle \tag{45}$$

and

$$\Psi(\vec{r}) = \psi_r(r)Y_{l,m}(\theta,\phi), \tag{46}$$

where

$$Y_{l,m}(\theta,\phi) = \langle\theta,\phi|l,m\rangle \tag{47}$$

denotes the standard spherical harmonic. A derivation of the spherical harmonic in a representation-independent way using the rotation operators of the "north-pole" state can be found in Ref. 7. The radial wavefunction is thus given by

$$\psi_r(r) = \langle r|\psi_r\rangle = \langle r=0|e^{\frac{i}{\hbar}r\left(p_r + i\frac{\hbar}{r}\right)}|\psi_r\rangle. \tag{48}$$

This is the relation that we will use to determine the radial wavefunctions for the three-dimensional hydrogen atom.

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We now turn to the expression of the two-dimensional translation operator in plane polar coordinates. In terms of Cartesian coordinates, we have

$$\widehat{T}(\vec{\rho}) = e^{-\frac{i}{\hbar}\vec{\rho}\cdot\hat{\vec{p}}} = e^{-\frac{i}{\hbar}\left(r_x\hat{p}_x + r_y\hat{p}_y\right)}, \tag{49}$$

with

$$\vec{\rho} = \vec{e}_x r_x + \vec{e}_y r_y, \ \hat{\vec{p}} = \vec{e}_x\hat{p}_x + \vec{e}_y\hat{p}_y. \tag{50}$$

We use $|0_{\vec{\rho}}\rangle$ as the position-space eigenvector at the origin for this two-dimensional case. We thus have

$$|\vec{\rho}\rangle = \widehat{T}(\vec{\rho})\ |0_{\vec{\rho}}\rangle. \tag{51}$$

Probably the simplest way to go from $|0_{\vec{\rho}}\rangle$ to $|\vec{\rho}\rangle$ is to translate by ρ in the $+x$-direction and then rotate by ϕ about the $+z$-direction. Indeed, this is the usual way of defining plane polar coordinates, ρ and ϕ. The corresponding operator is

$$\widehat{T}(\vec{\rho}) = e^{-\frac{i}{\hbar}\phi\hat{L}_z} e^{-\frac{i}{\hbar}\rho\hat{p}_x} e^{\frac{i}{\hbar}\phi\hat{L}_z}. \tag{52}$$

To show that this is correct, we use the braiding relation to obtain

$$\widehat{T}(\vec{\rho}) = e^{-\frac{i}{\hbar}\rho\left(\hat{p}_x\ \cos\phi + \hat{p}_y\ \sin\phi\right)}. \tag{53}$$

Since

$$r_x = \rho\ \cos\phi \quad \text{and} \quad r_y = \rho\ \sin\phi, \tag{54}$$

we immediately see that Eq. (53) reduces to Eq. (49).

From Eqs. (A22) and (A23), we obtain

$$\hat{p}_x = \left(\hat{p}_\rho - i\frac{\hbar}{2\,\hat{\rho}}\right)\cos\hat{\phi} - \hat{p}_\phi\ \sin\hat{\phi} \tag{55}$$

and

$$\hat{p}_y = \left(\hat{p}_\rho - i\frac{\hbar}{2\,\hat{\rho}}\right)\sin\hat{\phi} + \hat{p}_\phi\ \cos\hat{\phi}. \tag{56}$$

We use Eqs. (52) and (55) to write

$$\widehat{T}(\vec{\rho}) = e^{-\frac{i}{\hbar}\phi\hat{L}_z} e^{-\frac{i}{\hbar}\rho\left[\left(\hat{p}_\rho - i\frac{\hbar}{2\,\hat{\rho}}\right)\cos\hat{\phi} - \hat{p}_\phi\ \sin\hat{\phi}\right]} e^{\frac{i}{\hbar}\phi\hat{L}_z}. \tag{57}$$

We note that this is an operator identity.

A second way to express $\widehat{T}(\vec{\rho})$ in plane polar coordinates is simply to use Eqs. (54)–(56) to substitute for the Cartesian quantities in Eq. (49). In this way, we obtain

$$r_x\hat{p}_x + r_y\hat{p}_y = \rho\left[\left(\hat{p}_r - i\frac{\hbar}{2\,\hat{\rho}}\right)(\cos\phi\ \cos\hat{\phi} + \sin\phi\ \sin\hat{\phi}) - \hat{p}_\phi(\cos\phi\ \sin\hat{\phi} - \sin\phi\ \cos\hat{\phi})\right], \tag{58}$$

$$r_x\hat{p}_x + r_y\hat{p}_y = \rho\left[\left(\hat{p}_r - i\frac{\hbar}{2\,\hat{\rho}}\right)\cos(\hat{\phi} - \phi) - \hat{p}_\phi\ \sin(\hat{\phi} - \phi)\right], \tag{59}$$

and

$$r_x\hat{p}_x + r_y\hat{p}_y = e^{-\frac{i}{\hbar}\phi\hat{L}_z}\rho\left[\left(\hat{p}_r - i\frac{\hbar}{2\,\hat{\rho}}\right)\cos\hat{\phi} - \hat{p}_\phi\ \sin\hat{\phi}\right] e^{\frac{i}{\hbar}\phi\hat{L}_z}. \tag{60}$$

Upon substitution of this into Eq. (49), we immediately obtain Eq. (57).

Next, we determine how the general operator form of the translation operator in plane polar coordinates simplifies when it acts on the origin state in two dimensions, $|0_{\vec{\rho}}\rangle$, similar to what we did in the three-dimensional case.

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We introduce the same pair of $\vec{\delta}$-dependent exponentials to the left of $\widehat{T}(\vec{\rho})$, where $\vec{\delta}$ is a two-dimensional vector along $\vec{\rho}$, move the rightmost exponential factor to the right through $\widehat{T}(\vec{\rho})$, and operate on $|0_{\vec{\rho}}\rangle$. We thus obtain

$$|\vec{\rho}\rangle = e^{\frac{i}{\hbar}\vec{\delta}\cdot\hat{\vec{p}}}\widehat{T}(\vec{\rho})|\delta_x,\delta_y\rangle. \tag{61}$$

The choice that $\vec{\delta}$ lies along the same direction as $\vec{\rho}$ implies that Eq. (29) holds and

$$e^{\frac{i}{\hbar}\phi\hat{L}_z}|\delta_x,\delta_y\rangle = |\delta,0\rangle, \tag{62}$$

where δ is given by Eq. (33) with $\delta_z = 0$. Note that

$$\cos\hat{\phi}|\delta,0\rangle = \frac{\hat{r}_x}{\hat{\rho}}|\delta,0\rangle = |\delta,0\rangle \tag{63}$$

and

$$\sin\hat{\phi}|\delta,0\rangle = \frac{\hat{r}_y}{\hat{\rho}}|\delta,0\rangle = 0. \tag{64}$$

We expand the exponential containing $\hat{p}_\rho$ in Eq. (57) and use the action of $\cos\hat{\phi}$ and $\sin\hat{\phi}$ on $|\delta,0\rangle$ to simplify each term and then re-sum to obtain $\exp\left[-\frac{i}{\hbar}\rho\left(\hat{p}_\rho - i\frac{\hbar}{2\hat{\rho}}\right)\right]$ acting on the ket. This yields

$$|\vec{\rho}\rangle = e^{\frac{i}{\hbar}\vec{\delta}\cdot\hat{\vec{p}}}e^{-\frac{i}{\hbar}\phi\hat{L}_z}e^{-\frac{i}{\hbar}\rho\left(\hat{p}_\rho - i\frac{\hbar}{2\hat{\rho}}\right)}|\delta,0\rangle. \tag{65}$$

Since $\hat{L}_z$ commutes with $\hat{p}_\rho$ and $\hat{\rho}$, we can separate the radial and angular degrees of freedom according to

$$|\delta_x,\delta_y\rangle = e^{-\frac{i}{\hbar}\phi\hat{L}_z}|\delta,0\rangle = |\rho=\delta\rangle\otimes|\phi\rangle. \tag{66}$$

We define the radial coordinate eigenstate to satisfy

$$\hat{\rho}|\rho\rangle = \rho|\rho\rangle. \tag{67}$$

A direct calculation gives $\hat{\rho}|\delta_x,\delta_y\rangle = \delta|\delta_x,\delta_y\rangle$ justifying the label $\rho = \delta$ in Eq. (66). We similarly define the angular state, $|\phi\rangle$, to be the state that satisfies

$$\cos\hat{\phi}|\phi\rangle = \cos\phi|\phi\rangle, \quad \sin\hat{\phi}|\phi\rangle = \sin\phi|\phi\rangle. \tag{68}$$

Note that the operators $\hat{r}_x$ and $\hat{r}_y$ cannot operate solely on the states $|\rho\rangle$ or $|\phi\rangle$; that is, the domain of those operators lies outside of the space of the eigenstates of the radial-position operator $\hat{\rho}$ and of the angle ket $|\phi\rangle$. Of course, they can act on the tensor-product state $|\rho\rangle\otimes|\phi\rangle$ by decomposing the Cartesian position operators into their polar coordinate counterparts.

However, the operator $\hat{\rho}$ does act only on $|\rho\rangle$, which is its eigenstate, and it acts as the identity operator on $|\phi\rangle$. Similarly, $\cos\hat{\phi}$ and $\sin\hat{\phi}$ act nontrivially on $|\phi\rangle$, but as the identity on $|\rho\rangle$, as derived below. Consider $\cos\hat{\phi}$ acting on the state $|\rho\cos\phi,\rho\sin\phi\rangle = |\rho\rangle\otimes|\phi\rangle$, which is given by

$$\begin{aligned}\cos\hat{\phi}|\rho\rangle\otimes|\phi\rangle &= \frac{\hat{r}_x}{\hat{\rho}}|\rho\rangle\otimes|\phi\rangle \\ &= \hat{r}_x e^{-\frac{i}{\hbar}\phi\hat{L}_z}\frac{1}{\hat{\rho}}|\rho,0\rangle \\ &= e^{-\frac{i}{\hbar}\phi\hat{L}_z}\underbrace{e^{\frac{i}{\hbar}\phi\hat{L}_z}\hat{r}_x e^{-\frac{i}{\hbar}\phi\hat{L}_z}}_{\text{braiding}}\frac{1}{\hat{\rho}}|\rho,0\rangle \\ &= e^{-\frac{i}{\hbar}\phi\hat{L}_z}\frac{\cos\phi\hat{r}_x - \sin\phi\hat{r}_y}{\hat{\rho}}|\rho,0\rangle \\ &= \cos\phi|\rho\rangle\otimes|\phi\rangle.\end{aligned} \tag{69}$$

Note that the eigenvalue–eigenvector relationship given above is unchanged when we change the value of ρ in the radial ket. Hence, the operator $\cos\hat{\phi}$ acts as the identity on the $|\rho\rangle$ ket and can be taken to act solely on the $|\phi\rangle$ ket, yielding $\cos\hat{\phi}|\phi\rangle = \cos\phi|\phi\rangle$. Similarly, this separation also holds for $\sin\hat{\phi}$. The argument for the radial operator acting only on $|\rho\rangle$ can be verified by a similar argument.

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We now take the limit $\delta \to 0^+$ so that $\exp\left(\frac{i}{\hbar}\vec{\delta}\cdot\hat{\vec{p}}\right) \to 1$. Gathering the final results together, we have established that

$$|\vec{\rho}\rangle = e^{-\frac{i}{\hbar}\rho\left(\hat{p}_\rho - i\frac{\hbar}{2\,\rho}\right)}|\rho = 0\rangle \otimes |\phi\rangle \tag{70}$$

and

$$\langle\vec{\rho}| = \langle\phi| \otimes \langle\rho = 0|e^{\frac{i}{\hbar}\rho\left(\hat{p}_\rho + i\frac{\hbar}{2\,\rho}\right)}. \tag{71}$$

These final expressions are the simplification of the translation operator in plane polar coordinates that we sought when it acts on the state at the origin.

To calculate an energy wavefunction in position space, we decompose the energy eigenstate of the Hamiltonian into the tensor product of a radial state and an eigenstate of $\hat{L}_z$. This is given by

$$|\Psi\rangle = |\psi_\rho\rangle \otimes |m\rangle, \tag{72}$$

with $\hat{L}_z|m\rangle = \hbar m|m\rangle$. The wavefunction is then expressed as the product of a radial wavefunction and a z-component of angular momentum eigenfunction according to

$$\langle\vec{\rho}|\Psi\rangle = \langle\rho|\psi_\rho\rangle\langle\phi|m\rangle \tag{73}$$

or

$$\Psi(\vec{\rho}) = \psi_\rho(\rho)Y_m(\phi). \tag{74}$$

Here,

$$Y_m(\phi) = \langle\phi|m\rangle = \langle\phi = 0|e^{\frac{i}{\hbar}\hat{L}_z}|m\rangle = \langle\phi = 0|m\rangle e^{im\phi} = \frac{e^{im\phi}}{\sqrt{2\,\pi}} \tag{75}$$

denotes the standard eigenfunction of $\hat{L}_z$. We used the fact that normalization requires $\langle\phi = 0|m\rangle = 1/\sqrt{2\pi}$. The radial wavefunction is then given by

$$\psi_\rho(r) = \langle\rho|\psi_\rho\rangle = \langle\rho = 0|e^{\frac{i}{\hbar}\rho\left(\hat{p}_\rho + i\frac{\hbar}{2\,\rho}\right)}|\psi_\rho\rangle. \tag{76}$$

This is the relation that we use to determine the radial wavefunctions for the two-dimensional hydrogen atom in Sec. III.

III. APPLICATION OF THE FORMALISM TO THE COULOMB PROBLEM

We now show how these translation operators can be used to calculate wavefunctions of the Coulomb problem in three and two dimensions. We start in three dimensions, where we have

$$\hat{\mathscr{H}}^{3d} = \frac{\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2}{2\,\mu} - \frac{e^2}{\hat{r}}. \tag{77}$$

Here, μ is the reduced mass for the atom and $\mp e$ are the electronic and nuclear charges, respectively. Using the decomposition of the kinetic energy into radial and angular degrees of freedom, we find that the Hamiltonian can be re-written as

$$\hat{\mathscr{H}}^{3d} = \frac{\hat{p}_r^2}{2\,\mu} + \frac{\hat{\vec{L}}\cdot\hat{\vec{L}}}{2\,\mu\hat{r}^2} - \frac{e^2}{\hat{r}}. \tag{78}$$

We use a tensor product to represent the state vector in terms of the angular momentum eigenstate, $|l, m\rangle$, and the radial state $|\psi_r\rangle$ via $|\psi\rangle = |\psi_r\rangle \otimes |l, m\rangle$. Then, because $\hat{\vec{L}}\cdot\hat{\vec{L}}|l, m\rangle = \hbar^2 l(l+1)|l, m\rangle$, we have

$$\begin{aligned}\hat{\mathscr{H}}^{3d}(|\psi_r\rangle \otimes |l, m\rangle) &= \left[\frac{\hat{p}_r^2}{2\,\mu} + \frac{\hbar^2 l(l+1)}{2\,\mu\hat{r}^2} - \frac{e^2}{\hat{r}}\right]|\psi_r\rangle \otimes |l, m\rangle \\ &= \left(\hat{\mathscr{H}}_l^{3d}|\psi_r\rangle\right) \otimes |l, m\rangle,\end{aligned} \tag{79}$$

which defines the Hamiltonian $\hat{\mathscr{H}}_l^{3d}$ for a specific angular momentum sector. This Hamiltonian acts only on the radial part of the state vector because all terms in $\hat{\mathscr{H}}_l^{3d}$ commute with $\hat{\vec{L}}$.

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The Schrödinger factorization method is used to factorize each of these angular-momentum-sector Hamiltonians via

$$\hat{\mathscr{H}}_l^{3d} = \frac{\hat{p}_r^2}{2\,\mu} + \frac{\hbar^2 l(l+1)}{2\,\mu\hat{r}^2} - \frac{e^2}{\hat{r}} = \hat{B}_l^\dagger \hat{B}_l + E_l, \tag{80}$$

where the correct lowering operator satisfies

$$\hat{B}_l = \frac{1}{\sqrt{2\,\mu}}\left\{\hat{p}_r - i\hbar\left[\frac{1}{(l+1)a_0} - \frac{l+1}{\hat{r}}\right]\right\}, \tag{81}$$

which we can verify with the use of the commutation relation $[\hat{p}_r, \hat{r}^k] = -i\hbar k\hat{r}^{k-1}$ (which can be derived by induction from the radial momentum canonical commutation relation using the techniques in the Appendix). Note that the reason one can see for those two specific terms in $\hat{B}_l$ is that when we square the term in parentheses and when we commute it with $\hat{p}_r$, the resulting terms are always a constant term, a linear term in $1/\hat{r}$, and a quadratic term $(1/\hat{r}^2)$. By adjusting the coefficients, we can arrange for the product $\hat{B}_l^\dagger \hat{B}_l$ to have the required form. The symbol $a_0 = \frac{\hbar^2}{\mu e^2}$ is the Bohr radius, and $E_l = -\frac{e^2}{2(l+1)^2 a_0}$.

We denote the eigenstate of $\hat{\mathscr{H}}_l^{3d}$, corresponding to eigenvalue $E_{l=n-1}$ as $|n, l = n-1\rangle$. Here, n, which is a positive integer, is the standard principal quantum number, and the energy is degenerate for all l such that $0 \le l \le n-1$. We then have

$$E_{n-1} = -\frac{e^2}{2\,n^2 a_0}, \tag{82}$$

which, unfortunately, is conventionally denoted as E_n. To avoid confusion in the equations that follow, we do not redefine it, as is customarily done. Further note that the choice for the lowering operator in Eq. (81) was made so that the set of energies E_{n-1} form an *increasing sequence* for $1 \le n < \infty$. This choice for the increasing sequence guarantees that the eigenfunctions are all normalizable bound states.

Since $\hat{B}_l^\dagger \hat{B}_l$ is a non-negative semidefinite operator, it follows from Eq. (80) that the ground state $|n, n-1\rangle$ of $\hat{\mathscr{H}}_{n-1}^{3d}$ satisfies

$$\hat{\mathscr{H}}_{n-1}^{3d}|n, n-1\rangle = E_{n-1}|n, n-1\rangle, \tag{83}$$

with

$$\hat{B}_{n-1}|n, n-1\rangle = 0. \tag{84}$$

As we will see, this condition, which we term the *subsidiary condition*, facilitates the determination of all the eigenstates $|n, l\rangle$.

One can also directly verify that when the raising and lowering operators act in the "wrong" order, we have

$$\hat{B}_l\hat{B}_l^\dagger = \frac{\hat{p}_r^2}{2\,\mu} + \frac{\hbar^2(l+1)(l+2)}{2\,\mu\hat{r}^2} - \frac{e^2}{\hat{r}} - E_l = \hat{\mathscr{H}}_{l+1}^{3d} - E_l. \tag{85}$$

This allows us to derive the intertwining relationship when a $\hat{B}_l^\dagger$ operator is moved to the left past a $\hat{\mathscr{H}}_l^{3d}$ operator. In particular, we have

$$\begin{aligned}\hat{\mathscr{H}}_l^{3d}\hat{B}_l^\dagger &= \left(\hat{B}_l^\dagger \hat{B}_l + E_l\right)\hat{B}_l^\dagger \\ &= \hat{B}_l^\dagger \hat{B}_l\hat{B}_l^\dagger + E_l\hat{B}_l^\dagger \\ &= \hat{B}_l^\dagger\left(\hat{B}_l\hat{B}_l^\dagger + E_l\right) \\ &= \hat{B}_l^\dagger \hat{\mathscr{H}}_{l+1}^{3d}.\end{aligned} \tag{86}$$

Hence, when a $\hat{B}_l^\dagger$ operator starts on the right and moves to the left through $\hat{\mathscr{H}}_l^{3d}$, it shifts the index l of the Hamiltonian upward by one.

We use this intertwining identity to construct all the energy eigenstates that have energy E_{n-1}. Note that this approach is different from the original Schrödinger approach. It is the simplest way to establish all the energy eigenstates. For each n, we can find a total of n states with different total angular momenta that are eigenstates. The key observation is that the following set of states are eigenstates:

$$|n, l\rangle = C_{nl}\hat{B}_l^\dagger \hat{B}_{l+1}^\dagger \ldots \hat{B}_{n-3}^\dagger \hat{B}_{n-2}^\dagger |n, n-1\rangle, \tag{87}$$

where $0 \le l \le n-1$: note that when $l = n-1$, there are *no* $\hat{B}^\dagger$ operators needed and when $l = 0$, the string runs from $l = n-2$ down to $l = 0$. In particular, there is *no* $\hat{B}_{-1}^\dagger$ operator because $E_l \to -\infty$ as $l \to -1$. This terminates the chain at $l = 0$. The number C_{nl} is a normalization constant,

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which we determine below. To prove that $|n,l\rangle$ is an eigenstate of energy E_{n-1}, we simply operate with $\hat{\mathscr{H}}_l^{3d}$ on $|n,l\rangle$. Using the intertwining relation, to move the $\mathscr{H}^{3d}$ operator to the right, increasing its index by one with every step, we find that

$$\begin{aligned}\hat{\mathscr{H}}_l^{3d}|n,l\rangle &= \hat{\mathscr{H}}_l^{3d} C_{nl}\hat{B}_l^\dagger \hat{B}_{l+1}^\dagger \ldots \hat{B}_{n-3}^\dagger \hat{B}_{n-2}^\dagger |n,n-1\rangle \\ &= C_{nl}\hat{B}_l^\dagger \hat{\mathscr{H}}_{l+1}^{3d} \hat{B}_{l+1}^\dagger \ldots \hat{B}_{n-3}^\dagger \hat{B}_{n-2}^\dagger |n,n-1\rangle \\ &= C_{nl}\hat{B}_l^\dagger \hat{B}_{l+1}^\dagger \ldots \hat{B}_{n-3}^\dagger \hat{\mathscr{H}}_{n-2}^{3d} \hat{B}_{n-2}^\dagger |n,n-1\rangle \\ &= C_{nl}\hat{B}_l^\dagger \hat{B}_{l+1}^\dagger \ldots \hat{B}_{n-3}^\dagger \hat{B}_{n-2}^\dagger \hat{\mathscr{H}}_{n-1}^{3d} |n,n-1\rangle \\ &= -\frac{e^2}{2n^2 a_0}|n,l\rangle \end{aligned} \tag{88}$$

since the state $|n,n-1\rangle$ is an eigenstate of $\hat{\mathscr{H}}_{n-1}^{3d}$ with eigenvalue $-e^2/2n^2a_0$. We see that for a given n, all the states $|n,l\rangle$, with $0 \le l \le n-1$, belong to the eigenvalue E_{n-1}. Hence, we have constructed eigenstates of each of the lth angular-momentum-sector Hamiltonians with $0 \le l \le n-1$. When we make a tensor product of such a state with an $|l,m\rangle$ angular momentum state, it becomes an eigenstate of the full Coulomb Hamiltonian.

Before further moving in the derivation, we illustrate schematically what the energy levels are and how the different eigenstates interrelate. This is depicted in Fig. 2.

We also use the intertwining relation to normalize the state and determine C_{nl}. This is done by simply computing the norm

$$1 = \langle n,l|n,l\rangle = |C_{nl}|^2 \langle n,n-1|\hat{B}_{n-2}\ldots \underbrace{\hat{B}_l\hat{B}_l^\dagger}\ldots \hat{B}_{n-2}^\dagger|n,n-1\rangle. \tag{89}$$

We start with the innermost pair of raising and lowering operators and note that $\hat{B}_l\hat{B}_l^\dagger = \hat{\mathscr{H}}_{l+1}^{3d} - E_l$. If we move this operator through to the right, increasing its index by one with each step, until it acts directly on the state $|n,n-1\rangle$, we see that the intertwining relation will convert the Hamiltonian to the one corresponding to $l = n-1$. This can be immediately evaluated against the state $|n,n-1\rangle$, yielding the eigenvalue E_{n-1}. The net effect is we remove the product of the two operators $\hat{B}_l\hat{B}_l^\dagger$ and replace it with the factor $(E_{n-1} - E_l)$. Repeating $n-l-2$ more times, we find that

$$C_{nl} = \frac{1}{\sqrt{\prod_{k=l}^{n-2}(E_{n-1}-E_k)}} \tag{90}$$

$$= \sqrt{\left(\frac{2a_0n^2}{e^2}\right)^{n-l-1}\frac{(n+l)![(n-1)!]^2}{(2n-1)!(n-l-1)!(l!)^2}}. \tag{91}$$

Note that this final result requires that the initial state $|n,n-1\rangle$ be normalized, i.e., $\langle n,n-1|n,n-1\rangle = 1$. We will ensure that this is true.

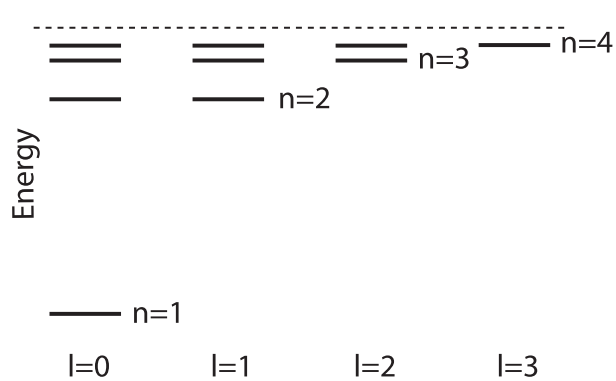

FIG. 2. Plot of the energy levels of the three-dimensional Coulomb problem up to $n = 4$. The states $|n,n-1\rangle$ are the rightmost states in each row. Each additional $\hat{B}^\dagger$ operator moves us one step to the left (there are no more $\hat{B}^\dagger$ operators to apply after $l = 0$). All energies in a given row are degenerate. The dashed line shows where $E = 0$.

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The next step is to show that the string of $\hat{B}^\dagger$ operators acting on $|n, n-1\rangle$ is proportional to a Laguerre polynomial in $\hat{r}$ (multiplied by a power of $1/\hat{r}$) acting on the same state. To do this, we need to go through a proof by induction. Our starting point is to observe that the subsidiary condition in Eq. (84) can be rewritten as

$$\hat{p}_r|n, n-1\rangle = i\hbar\left(\frac{1}{na_0} - \frac{n}{\hat{r}}\right)|n, n-1\rangle. \tag{92}$$

This allows us to replace the radial momentum operator acting on the state $|n, n-1\rangle$ by the sum of a constant and a term that goes like $1/\hat{r}$ (acting on the same state). Given that the commutation relation of the radial momentum with an inverse power of $\hat{r}$ increases the power by one as well, one can immediately see that the string of $\hat{B}^\dagger$ operators acting on $|n, n-1\rangle$ will be a polynomial of degree $n-l-1$ in $1/\hat{r}$. By factoring out $1/\hat{r}^{n-l-1}$, we are left with a polynomial of degree $n-l-1$ in $\hat{r}$. Recognizing that the dimensionality of a $\hat{B}^\dagger$ operator is $\hbar/(\sqrt{\mu}a_0)$ and using $2\hat{r}/na_0$ as the expansion parameter for the polynomial, we have that

$$\hat{B}_l^\dagger \ldots \hat{B}_{n-2}^\dagger|n, n-1\rangle = \left(\frac{2i\hbar}{\sqrt{2\mu}na_0}\right)^{n-l-1}\left(\frac{na_0}{2\hat{r}}\right)^{n-l-1}\sum_{j=0}^{n-l-1} b_j^{(l)}\left(\frac{2\hat{r}}{na_0}\right)^j|n, n-1\rangle. \tag{93}$$

Note that we are suppressing a label of n corresponding to the principal quantum number in the notation for the b coefficients to streamline the notation; one must remember that a set of b coefficients is generated for each principal quantum number n. We choose the base case to correspond to $l = n-2$, where the polynomial is just equal to

$$\begin{aligned}\hat{B}_{n-2}^\dagger|n, n-1\rangle &= \frac{i\hbar}{\sqrt{2\,\mu}}\left[\frac{2n-1}{n(n-1)a_0} - \frac{2n-1}{\hat{r}}\right]|n, n-1\rangle \\ &= \left(\frac{2i\hbar}{\sqrt{2\mu}na_0}\right)\left(\frac{na_0}{2\hat{r}}\right)\left[-2n+1+\frac{2n-1}{2(n-1)}\left(\frac{2\hat{r}}{na_0}\right)\right]|n, n-1\rangle,\end{aligned} \tag{94}$$

so that $b_0^{(n-2)} = -2n+1$ and $b_1^{(n-2)} = (2n-1)/2(n-1)$. (One could have taken the base case as $l = n-1$, with $b_0^{(n-1)} = 1$, but we chose not to because that is a trivial base case.) To evaluate the induction step, we remove the leftmost $\hat{B}_l^\dagger$ and collect what remains in terms of the polynomial for $l+1$. Then, we operate the $\hat{p}_r$ operator to the right, commuting it through the $\hat{r}$ operators until it can act on the state $|n, n-1\rangle$, where we can use Eq. (92) to replace it by a binomial in $1/\hat{r}$. After collecting the coefficients of powers of $\hat{r}$, we find that

$$\sum_{j=0}^{n-l-1} b_j^{(l)}\left(\frac{2\hat{r}}{na_0}\right)^j = \sum_{j=0}^{n-l-1}\left(\frac{2\hat{r}}{na_0}\right)^j\left[-(j+2l+3)b_j^{(l+1)} + \frac{n+l+1}{2(l+1)}b_{j-1}^{(l+1)}\right], \tag{95}$$

where we set $b_{-1}^{(l+1)} = b_{n-l-1}^{(l+1)} = 0$. The key to determining that these results yield associated Laguerre polynomials is to compute the ratio of successive coefficients of the lth polynomial using the two formulas we have. This gives

$$\frac{b_{j+1}^{(l)}}{b_j^{(l)}} = \frac{(j+2l+4)\left(\frac{b_{j+1}^{(l+1)}}{b_j^{(l+1)}}\right) - \frac{n+l+1}{2(l+1)}}{(j+2l+3) - \frac{n+l+1}{2(l+1)}\left(\frac{b_j^{(l+1)}}{b_{j-1}^{(l+1)}}\right)^{-1}} \qquad \text{for} \quad 0 \le j \le n-l-2. \tag{96}$$

Here, again, we note that $b_{-1}^{(l+1)} = b_{n-l-1}^{(l+1)} = 0$. This brings us to the induction hypothesis. The ratio is given by

$$\frac{b_{j+1}^{(l)}}{b_j^{(l)}} = \frac{j-n+l+1}{(j+1)(j+2l+2)}. \tag{97}$$

One can immediately see from Eq. (94), for $l = n-2$, that the base case gives $b_1^{(n-2)}/b_0^{(n-2)} = -1/2(n-1)$, which agrees with the induction hypothesis in Eq. (97) for $l = n-2$ and $j = 0$. Hence, we assume that it holds for $l+1$ and substitute into Eq. (96) to show it holds for l. This yields

$$\frac{b_{j+1}^{(l)}}{b_j^{(l)}} = \frac{\frac{(j-n+l+2)}{(j+1)} - \frac{(n+l+1)}{2(l+1)}}{(j+2l+3)\left[1 - \frac{(n+l+1)j}{2(l+1)(j-n+l+1)}\right]}. \tag{98}$$

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Putting everything over common denominators yields

$$\frac{b_{j+1}^{(l)}}{b_j^{(l)}} = \frac{(j-n+l+1)[2(l+1)(j-n+l+2)-(j+1)(n+l+1)]}{(j+2l+3)(j+1)[2(l+1)(j-n+l+1)-j(n+l+1)]}. \tag{99}$$

Expanding the terms in the numerator and denominator in the square brackets, factorizing the expansion, and simplifying then reduces this result to the one in Eq. (97), which establishes the induction proof. It turns out that the coefficients of a polynomial that satisfy Eq. (97) are associated Laguerre functions. We use the definition of the associated Laguerre function given by Powell and Crasemann in their quantum mechanics textbook,[8]

$$L_k^{\alpha}(x) = \sum_{j=0}^{m} \frac{(-1)^j}{j!}\binom{k+\alpha}{k-j} x^j = \sum_{j=0}^{k} a_j^{(\alpha,k)} x^j, \tag{100}$$

which defines the coefficients of the polynomial $a_j^{(\alpha,k)}$. We immediately see from Eq. (100) that

$$\frac{a_{j+1}^{(\alpha,k)}}{a_j^{(\alpha,k)}} = \frac{j-k}{(j+1)(\alpha+j+1)}. \tag{101}$$

This then tells us that the polynomial given by the string of $\hat{B}^\dagger$ operators acting on $|n, n-1\rangle$ is *proportional* to the associated Laguerre function with argument given by $2\hat{r}/na_0$, $\alpha = 2l+1$, and $k = n-l-1$. To find the constant of proportionality [in addition to the power $(2\hat{r}/na_0)^{n-l-1}$, which we already knew from Eq. (93)], we evaluate the constant term (no $\hat{r}$ dependence or the maximal power of $\hat{r}$ in the sum) in Eq. (93). It is given by

$$\left(\frac{2i\hbar}{\sqrt{2\mu}na_0}\right)^{n-l-1} b_{n-l-1}^{(l)} = \left(\frac{i\hbar}{\sqrt{2\,\mu}}\right)^{n-l-1} \prod_{k=l+1}^{n-1}\left(\frac{1}{na_0}+\frac{1}{ka_0}\right), \tag{102}$$

where the right-hand side is found from the constant terms in each $\hat{B}^\dagger$ and from each $\hat{p}_r$ in each $\hat{B}^\dagger$ when it acts on $|n, n-1\rangle$. This constant term is not modified by the commutators of the radial momentum with inverse powers of $\hat{r}$. From this, we learn that

$$b_{n-l+1}^{(l)} = \left(\frac{1}{2}\right)^{n-l-1} \frac{l!(2n-1)!}{(n-1)!(n+l)!}. \tag{103}$$

However, if we instead express $b_{n-l-1}^{(l)}$ in terms of the maximal coefficient of the Laguerre polynomial, we find that

$$b_{n-l+1}^{(l)} = C' a_{n-l-1}^{(2l+1,n-l-1)} = C' \frac{(-1)^{n-l-1}}{(n-l-1)!}, \tag{104}$$

where C' is the proportionality constant we need to determine. We immediately learn that

$$C' = \left(-\frac{1}{2}\right)^{n-l-1} \frac{l!(n-l-1)!(2n-1)!}{(n+l)!(n-1)!}. \tag{105}$$

Putting this all together, we have derived the identity that

$$\begin{aligned}\hat{B}_l^\dagger \hat{B}_{l+1}^\dagger \ldots \hat{B}_{n-3}^\dagger \hat{B}_{n-2}^\dagger |n, n-1\rangle = &\left(-\frac{i\hbar}{\sqrt{2\mu}na_0}\right)^{n-l-1} \frac{l!(n-l-1)!(2n-1)!}{(n+l)!(n-1)!} \\ &\times \left(\frac{na_0}{2\hat{r}}\right)^{n-l-1} L_{n-l-1}^{2l+1}\left(\frac{2\hat{r}}{na_0}\right)|n, n-1\rangle.\end{aligned} \tag{106}$$

Finally, we multiply by C_{nl} from Eq. (91) and find that

$$|n, l\rangle = (-i)^{n-l-1}\sqrt{\frac{(n-l-1)!(2n-1)!}{(n+l)!}}\left(\frac{na_0}{2\hat{r}}\right)^{n-l-1} L_{n-l-1}^{2l+1}\left(\frac{2\hat{r}}{na_0}\right)|n, n-1\rangle. \tag{107}$$

Since the eigenvector is defined only up to a complex phase, we choose to remove the factor of $(-i)^{n-l-1}$ in the following.

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We are now ready to compute the wavefunction. We take the overlap of the position eigenstate with the energy eigenstate or

$$(\langle\theta\phi| \otimes \langle r|)(|n,l\rangle \otimes |l,m\rangle). \tag{108}$$

Using the fact that[7]

$$Y_{lm} = \langle\theta\phi|lm\rangle, \tag{109}$$

we find that

$$\psi_{nlm}(r,\theta,\phi) = \sqrt{\frac{(n-l-1)!(2n-1)!}{(n+l)!}}\langle r|\left(\frac{na_0}{2\hat{r}}\right)^{n-l-1} L_{n-l-1}^{2l+1}\left(\frac{2\hat{r}}{na_0}\right)|n,n-1\rangle Y_{lm}(\theta,\phi). \tag{110}$$

Because $\hat{r}|r\rangle = r|r\rangle$, we immediately find that

$$\psi_{nlm}(r,\theta,\phi) = \sqrt{\frac{(n-l-1)!(2n-1)!}{(n+l)!}}\langle r|n,n-1\rangle\left(\frac{na_0}{2r}\right)^{n-l-1} L_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right)Y_{lm}(\theta,\phi). \tag{111}$$

What remains is to determine the first wavefunction in the chain, $\phi_n(r) = \langle r|n,n-1\rangle$. This is where we need to use the translation operator in spherical coordinates. The radial translation operator is an exponential of $i\,r\left(\hat{p}_r + \frac{i\hbar}{\hat{r}}\right)/\hbar$ when acting on the position eigenvector at the origin. While one can evaluate the exponential of an operator acting on a state via expanding the power series term by term, a more efficient evaluation can be accomplished if one evaluates the operator acting on one of its eigenvectors—then, the exponentiation becomes trivial. This is the strategy we adopt here.

We start with some additional operator identities. First, note that $[\hat{p}_r, \hat{r}^{-n+1}] = i\hbar(n-1)/\hat{r}^n$. (See the Appendix for details.) Hence, we use Eq. (92) and the commutator to find that

$$\hat{p}_r\frac{1}{\hat{r}^{n-1}}|n,n-1\rangle = i\hbar\left(\frac{1}{na_0\hat{r}^{n-1}} - \frac{1}{\hat{r}^n}\right)|n,n-1\rangle, \tag{112}$$

or

$$\left(\hat{p}_r + \frac{i\hbar}{\hat{r}}\right)\frac{1}{\hat{r}^{n-1}}|n,n-1\rangle = \frac{i\hbar}{na_0}\frac{1}{\hat{r}^{n-1}}|n,n-1\rangle. \tag{113}$$

Note that this says that the state $(1/\hat{r}^{n-1})|n,n-1\rangle$ is an eigenvector for the operator $\left(\hat{p}_r + \frac{i\hbar}{\hat{r}}\right)$ with eigenvalue $i\hbar/na_0$. An imaginary eigenvalue is possible because this operator is *not* Hermitian.

We are now ready to use the translation operator in spherical coordinates. Since $\langle\theta\phi| = \langle 0,0,1|\exp(i\theta\hat{L}_y/\hbar)\exp(i\phi\hat{L}_z/\hbar)$, we have that

$$\langle r| = \langle 0_r|\exp\left[\frac{ir}{\hbar}\left(\hat{p}_r + \frac{i\hbar}{\hat{r}}\right)\right]. \tag{114}$$

The wavefunction $\phi_n(r)$ then becomes

$$\begin{aligned}\phi_n(r) = \langle r|n,n-1\rangle &= \langle r|\frac{\hat{r}^{n-1}}{\hat{r}^{n-1}}|n,n-1\rangle = r^{n-1}\langle r|\frac{1}{\hat{r}^{n-1}}|n,n-1\rangle \\ &= r^{n-1}\langle 0_r|\exp\left[\frac{ir}{\hbar}\left(\hat{p}_r + \frac{i\hbar}{\hat{r}}\right)\right]\frac{1}{\hat{r}^{n-1}}|n,n-1\rangle.\end{aligned} \tag{115}$$

Because the state on the right is an eigenvector for $\left(\hat{p}_r + \frac{i\hbar}{\hat{r}}\right)$, we immediately find that

$$\phi_n(r) = r^{n-1}\exp\left(-\frac{r}{na_0}\right)\langle 0_r|\frac{1}{\hat{r}^{n-1}}|n,n-1\rangle. \tag{116}$$

Note that the term $\langle 0_r|\frac{1}{\hat{r}^{n-1}}|n,n-1\rangle$ is a constant because Eq. (116) shows that

$$\lim_{r\to 0}\frac{1}{r^{n-1}}\phi_n(r) = \langle 0_r|\frac{1}{\hat{r}^{n-1}}|n,n-1\rangle. \tag{117}$$

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Its precise value is determined by normalization. We find that

$$1 = \left(\langle 0_r|\frac{1}{\hat{r}^{n-1}}|n, n-1\rangle\right)^2 \int_0^\infty dr\, r^{2n} e^{-\frac{2r}{na_0}}, \tag{118}$$

which yields

$$\phi_n(r) = \left(\frac{2}{na_0}\right)^{n+\frac{1}{2}} \frac{1}{\sqrt{(2n)!}} r^{n-1} \exp\left(-\frac{r}{na_0}\right). \tag{119}$$

While this result can be calculated in many different ways, one cannot calculate this wavefunction using the translation operator in Cartesian coordinates; the translation operator must be expressed in terms of spherical coordinates because it involves a power series in r that includes odd powers.

We can now summarize our final wavefunction by combining all our results together,

$$\psi_{nlm}(r,\theta,\phi) = \left(\frac{2}{na_0}\right)^{\frac{3}{2}} \sqrt{\frac{(n-l-1)!}{2n(n+l)!}} \left(\frac{2r}{na_0}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right) e^{-\frac{r}{na_0}} Y_{lm}(\theta,\phi), \tag{120}$$

which is the standard result for the three-dimensional Coulomb bound-state wavefunctions using the Laguerre polynomial definition in Eq. (100). We want to stress that the entire calculation was based on the representation-independent approach described in the introduction. All the steps in the derivation used operator algebra. We never needed to represent momentum operators in terms of spatial derivatives. It is comforting to know that wavefunctions *can* be calculated in such a representation-independent way.

Having completed our first example, we now move on to the second. We will expedite the description because many of the techniques for the two-dimensional case are similar to those of the three-dimensional case. However, the two-dimensional case does illustrate some interesting new twists, so it is important to describe it carefully.

The Coulomb Hamiltonian in two dimensions is given by

$$\hat{\mathscr{H}}^{2d} = \frac{\hat{p}_x^2 + \hat{p}_y^2}{2\mu} - \frac{e^2}{\hat{\rho}}. \tag{121}$$

The kinetic energy can again be decomposed into radial and angular components (see the Appendix),

$$\mathscr{H}^{2d} = \frac{\hat{p}_\rho^2}{2\mu} + \frac{\hat{L}_z^2 - \frac{\hbar^2}{4}}{2\mu\hat{\rho}^2} - \frac{e^2}{\hat{\rho}}, \tag{122}$$

with

$$\hat{p}_\rho = \frac{1}{\hat{\rho}}\left(\hat{r}_x\hat{p}_x + \hat{r}_y\hat{p}_y - \frac{i\hbar}{2}\right). \tag{123}$$

Note that in two dimensions, we do have a quantum correction to the kinetic energy (given by the $-\hbar^2/8\mu\hat{\rho}^2$ term). Here, the angular momentum states are given by eigenstates of $\hat{L}_z$, which satisfy $\hat{L}_z|m\rangle = \hbar m|m\rangle$. Therefore, we form the energy eigenstates as a tensor product of radial and angular momentum states via $|\psi\rangle = |\psi_\rho\rangle \otimes |m\rangle$. Operating the Hamiltonian onto the tensor-product state yields

$$\begin{aligned}\mathscr{H}^{2d}(|\psi_\rho\rangle \otimes |m\rangle) &= \left[\frac{\hat{p}_\rho^2}{2\mu} + \frac{\hbar^2(m^2 - \frac{1}{4})}{2\mu\hat{\rho}^2} - \frac{e^2}{\hat{\rho}}\right]|\psi_\rho\rangle \otimes |m\rangle \\ &= \left(\mathscr{H}_m^{2d}|\psi_\rho\rangle\right) \otimes |m\rangle,\end{aligned} \tag{124}$$

where the second line defines the set of Hamiltonians, $\mathscr{H}_m^{2d}$, that operate only on the radial state $|\psi_\rho\rangle$. Note here that the index m can be a positive or negative integer, unlike in the three-dimensional case, where l is a non-negative integer. Since each of these Hamiltonians depends on m only through m^2, we immediately learn that the radial eigenfunctions and the energy eigenvalues depend only on the magnitude of m, that is, on $|m|$.

We continue to use the Schrödinger factorization method for $m \geq 0$ via

$$\mathscr{H}_m^{2d} = \frac{\hat{p}_\rho^2}{2\mu} + \frac{\hbar^2\left(m^2 - \frac{1}{4}\right)}{2\mu\hat{\rho}^2} - \frac{e^2}{\hat{\rho}} = \hat{B}_m^\dagger \hat{B}_m + E_m. \tag{125}$$

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A quick calculation tells us that

$$\hat{B}_m = \frac{1}{\sqrt{2\mu}}\left\{\hat{p}_\rho - i\hbar\left[\frac{1}{\left(m+\frac{1}{2}\right)a_0} - \frac{\left(m+\frac{1}{2}\right)}{\hat{\rho}}\right]\right\} \tag{126}$$

and

$$E_m = -\frac{e^2}{2a_0\left(m+\frac{1}{2}\right)^2}. \tag{127}$$

Note that for $m \geq 0$, the energies form an increasing sequence, which is required for all the energy eigenstates to be normalizable. While the algebra above holds for all m, we first focus on working with non-negative m; we will describe how to handle negative m later. In particular, we already know that the radial part of the eigenvectors will be identical, as will the energies, so we will not be using the above formulas with negative m to solve these problems.

Computing the product of the two operators in opposite order gives us

$$\hat{B}_m\hat{B}_m^\dagger + E_m = \frac{\hat{p}_\rho^2}{2\mu} + \frac{\hbar^2\left[(m+1)^2 - \frac{1}{4}\right]}{2\mu\hat{\rho}^2} - \frac{e^2}{\hat{\rho}} = \mathscr{H}_{m+1}^{2d}. \tag{128}$$

This relation is essentially the same relation as we had in three-dimensions, Eq. (85), so that we immediately find the corresponding intertwining relation (for $m \geq 0$)

$$\mathscr{H}_m^{2d}\hat{B}_m^\dagger = \hat{B}_m^\dagger\mathscr{H}_{m+1}^{2d}, \tag{129}$$

which can be employed to find eigenstates in the same fashion: we have the eigenvectors given by

$$|n,m\rangle = C_{nm}\hat{B}_m^\dagger\hat{B}_{m+1}^\dagger\ldots\hat{B}_{n-3}^\dagger\hat{B}_{n-2}^\dagger|n,n-1\rangle, \tag{130}$$

for $m \geq 0$, with the eigenvalues equal to

$$E_{n-1} = -\frac{e^2}{2a_0\left(n-\frac{1}{2}\right)^2} \tag{131}$$

and C_{nm} being a normalization constant. The state $|n, m = n-1\rangle = |n, n-1\rangle$ satisfies

$$\hat{B}_{n-1}|n,n-1\rangle = 0. \tag{132}$$

As seen in the three-dimensional case, the normalization constant (for $m \geq 0$) is given by

$$\begin{aligned} C_{nm} &= \frac{1}{\sqrt{\prod_{k=m}^{n-2}(E_{n-1}-E_k)}} \\ &= \left(\frac{\sqrt{a_0}\left(n-\frac{1}{2}\right)}{\sqrt{2}e}\right)^{n-m-1}\sqrt{\frac{(n+m-1)!\left[(2n-3)!!\right]^2}{(2n-2)!(n-m-1)!\left[(2m-1)!!\right]^2}}. \end{aligned} \tag{133}$$

We now discuss some interesting observations about what happens when $m < 0$. For example, one can see from Eq. (126) that $\hat{B}_{-|m|} = \hat{B}_{|m|-1}^\dagger$. Hence, if we extend the eigenstates in Eq. (130) for $m < 0$, then, because we have that

$$\begin{aligned} \hat{B}_{-|m|}^\dagger\ldots\hat{B}_{-1}^\dagger\hat{B}_0^\dagger\ldots\hat{B}_{|m|-1}^\dagger &= \hat{B}_{|m|-1}\ldots\underbrace{\hat{B}_0\hat{B}_0^\dagger}\ldots\hat{B}_{|m|-1}^\dagger \\ &= \hat{B}_{|m|-1}\ldots\hat{B}_1(\mathscr{H}_1^{2d}-E_0)\hat{B}_1^\dagger\ldots\hat{B}_{|m|-1}^\dagger \\ &= \hat{B}_{|m|-1}\ldots\hat{B}_1\hat{B}_1^\dagger\ldots\hat{B}_{|m|-1}^\dagger(\mathscr{H}_{|m|}^{2d}-E_0) \\ &= (\mathscr{H}_{|m|}^{2d}-E_{|m|-1})\ldots(\mathscr{H}_{|m|}^{2d}-E_0), \end{aligned} \tag{134}$$

we can show the equivalence of the radial component of the eigenvectors for negative m with positive m. If we let the product of operators in Eq. (134) act on $|n, |m|\rangle$, then each $\mathscr{H}_{|m|}^{2d}$ yields $E_{|m|}$, so we find that

$$|n,-|m|\rangle = |n,|m|\rangle \tag{135}$$

directly from the operator identities. This confirms our statement before that the radial component of the eigenvector for $-|m|$ is *identical* to the eigenvector for $|m|$ (with the same principal quantum number n). Further note that the product of numerical factors is precisely the numerical factors to guarantee that $C_{n-|m|} = C_{n|m|}$, which is why we have an equality in Eq. (135) rather than a proportionality.

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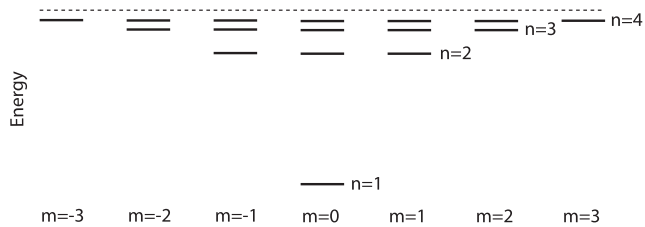

FIG. 3. Plot of the energy levels of the two-dimensional Coulomb problem up to $n = 4$. The states $|n, n-1\rangle$ are the rightmost states in each row. Each additional $\hat{B}^\dagger$ operator moves us one step to the left (there are no more $\hat{B}^\dagger$ operators to apply after $m = -n+1$). All energies in a given row are degenerate. The dashed line shows where $E = 0$.

At this stage, we show the spectra along with the operator representation of the radial components of the eigenvectors in Fig. 3. All the states in a horizontal row (fixed n, $-n+1 \le m \le n-1$) are degenerate with energy E_{n-1}. The column with $m = 0$ has the largest number of eigenstates. As $|m|$ increases, the number of total eigenstates decreases by 1 for each step moving further away from $m = 0$ (to the right or to the left).

Our next goal is to find the wavefunctions in position space, and we now assume $m \ge 0$ again. As mentioned before, we see that the string of $\hat{B}^\dagger$ operators acting on the state $|n, n-1\rangle$ will create a polynomial of degree $n-m-1$ in $1/\hat{\rho}$. If we factor out the term $1/\hat{\rho}^{n-m-1}$, then the polynomial is an order $n-m-1$ polynomial in $\hat{\rho}$. Just as we saw happen in three dimensions, it turns out to be a Laguerre polynomial for the two-dimensional case too.

To see this, we start with a definition of the coefficients of the nth polynomial (for $m \ge 0$, without loss of generality),

$$\hat{B}^\dagger_m \ldots \hat{B}^\dagger_{n-2}|n, n-1\rangle = \left[\frac{2i\hbar}{\sqrt{2\mu}\left(n-\frac{1}{2}\right)a_0}\right]^{n-m-1}\left[\frac{\left(n-\frac{1}{2}\right)a_0}{2\hat{\rho}}\right]^{n-m-1}\sum_{j=0}^{n-m-1} b_j^{(m)}\left[\frac{2\hat{\rho}}{\left(n-\frac{1}{2}\right)a_0}\right]^j |n, n-1\rangle. \tag{136}$$

Again, we suppress the index n in the labeling of the b coefficients for notational simplicity. We consider the base case first, corresponding to $m = n-2$. First, we need to determine a modification of the subsidiary condition in Eq. (132) to determine what happens when the radial momentum acts on $|n, n-1\rangle$,

$$\hat{p}_\rho|n, n-1\rangle = i\hbar\left[\frac{1}{\left(n-\frac{1}{2}\right)a_0} - \frac{n-\frac{1}{2}}{\hat{\rho}}\right]|n, n-1\rangle. \tag{137}$$

Next, we have that the base case is

$$\begin{aligned}\hat{B}^\dagger_{n-2}|n, n-1\rangle &= \frac{i\hbar}{\sqrt{2\mu}}\left[\frac{2n-2}{\left(n-\frac{1}{2}\right)\left(n-\frac{3}{2}\right)a_0} - \frac{2n-2}{\hat{\rho}}\right]|n, n-1\rangle \\ &= \left[\frac{2i\hbar}{\sqrt{2\mu}\left(n-\frac{1}{2}\right)a_0}\right]\left[\frac{\left(n-\frac{1}{2}\right)a_0}{2\hat{\rho}}\right]\left[-(2n-2) + \frac{2n-2}{2n-3}\frac{2\hat{\rho}}{\left(n-\frac{1}{2}\right)a_0}\right]|n, n-1\rangle\end{aligned} \tag{138}$$

so that $b_0^{(n-2)} = -(2n-2)$ and $b_1^{(n-2)} = (2n-2)/(2n-3)$. This means that $b_1^{(n-2)}/b_0^{(n-2)} = -1/(2n-3)$, a fact we shall use momentarily.

After establishing the base case for the proof by induction, we next examine the m-th polynomial by splitting off the operator $\hat{B}^\dagger_m$ and having it act on the $(m+1)$st polynomial. This yields

$$\sum_{j=0}^{n-m-1}\left[-(j+2m+2)b_j^{(m+1)} + \frac{m+n}{2m+1}b_{j-1}^{(m+1)}\right]\left[\frac{2\hat{\rho}}{\left(n-\frac{1}{2}\right)a_0}\right]^j = \sum_{j=0}^{n-m-1} b_j^{(m)}\left[\frac{2\hat{\rho}}{\left(n-\frac{1}{2}\right)a_0}\right]^j. \tag{139}$$

Then, we determine the ratio of subsequent coefficients of the polynomials, just like before, and find that

$$\frac{b_{j+1}^{(m)}}{b_j^{(m)}} = \frac{(j+2m+3)\left[\frac{b_{j+1}^{(m+1)}}{b_j^{(m+1)}}\right] - \frac{m+n}{2m+1}}{(j+2m+2) - \frac{m+n}{2m+1}\left[\frac{b_j^{(m+1)}}{b_{j-1}^{(m+1)}}\right]^{-1}} \qquad \text{for} \quad 0 \le j \le n-m-2, \tag{140}$$

where we again use $b_{-1}^{(m+1)} = b_{n-m-1}^{(m+1)} = 0$.

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The induction hypothesis is that

$$\frac{b_{j+1}^{(m)}}{b_j^{(m)}} = \frac{j-n+m+1}{(j+1)(j+2m+1)}. \tag{141}$$

Recalling the base case, with $m = n-2$ and $j = 0$, we have that the ratio equals $-1/(2n-3)$, which is what we already calculated above for the base case. Substituting the induction hypothesis for $m+1$ (evaluated for j and for $j-1$) into Eq. (140) yields

$$\frac{b_{j+1}^{(m)}}{b_j^{(m)}} = \frac{(j-n+m+1)[(2m+1)(j-n+m+2)-(m+n)(j+1)]}{(j+1)(j+2m+2)[(2m+1)(j-n+m+1)-(m+n)j]}. \tag{142}$$

Expanding the terms in the square brackets, factorizing them, and simplifying produces the results in Eq. (141), which completes the induction proof. Given the ratio of the consecutive coefficients in the Laguerre polynomial in Eq. (101), we see that the string of $B^\dagger$ operators acting on $|n, n-1\rangle$ yields the Laguerre polynomial (with $\alpha = 2m$ and $k = n-m-1$) multiplied by a power of $\hat{\rho}$ multiplied by a constant, or

$$\hat{B}_m^\dagger \cdots \hat{B}_{n-2}^\dagger |n, n-1\rangle = C'\left[\frac{2i\hbar}{\sqrt{2\,\mu}\left(n-\frac{1}{2}\right)a_0}\right]^{n-m-1}\left[\frac{\left(n-\frac{1}{2}\right)a_0}{2\hat{\rho}}\right]^{n-m-1} L_{n-m-1}^{2m}\left(\frac{2\hat{\rho}}{\left(n-\frac{1}{2}\right)a_0}\right)|n, n-1\rangle. \tag{143}$$

Using the same approach as described before, we compute the coefficient of the term that has no $\hat{\rho}$ dependence. We express the result in terms of the b coefficients and equate it to the constant term found from using the subsidiary condition when the string of $\hat{B}^\dagger$ operators acts on $|n, n-1\rangle$. We have

$$\left[\frac{2i\hbar}{\sqrt{2\,\mu}\left(n-\frac{1}{2}\right)a_0}\right]^{n-m-1} b_{n-m-1}^{(m)} = \left(\frac{i\hbar}{\sqrt{2\mu}}\right)^{n-m-1}\prod_{k=m}^{n-2}\left[\frac{1}{\left(n-\frac{1}{2}\right)a_0}+\frac{1}{\left(k+\frac{1}{2}\right)a_0}\right], \tag{144}$$

which can be solved for $b_{n-m-1}^{(m)}$ with

$$b_{n-m-1}^{(m)} = \frac{(2n-2)!(2m-1)!!}{(n+m-1)!(2n-3)!!}. \tag{145}$$

We also can calculate this coefficient from the Laguerre polynomial form. We have

$$b_{n-m-1}^{(m)} = C' a_{m-n-1}^{(2m,n-m-1)} = \frac{(-1)^{n-m-1}}{(n-m-1)!}. \tag{146}$$

Hence, we have

$$C' = (-1)^{n-m-1}\frac{(n-m-1)!(2n-2)!(2m-1)!!}{(n+m-1)!(2n-3)!!} \tag{147}$$

and

$$|n, m\rangle = (-i)^{n-m-1}\sqrt{\frac{(n-m-1)!(2n-2)!}{(n+m-1)!}}\left[\frac{\left(n-\frac{1}{2}\right)a_0}{2\hat{\rho}}\right]^{n-m-1} L_{n-m-1}^{2m}\left(\frac{2\hat{\rho}}{\left(n-\frac{1}{2}\right)a_0}\right)|n, n-1\rangle. \tag{148}$$

As mentioned before, we drop the irrelevant phase factor, $(-i)^{n-m-1}$. Now, we are ready to compute the wavefunctions. We need to determine the overlap of $\langle\phi| \otimes \langle\rho|$ with $|n, m\rangle \otimes |m\rangle$. Since $\langle\phi|m\rangle = \exp(im\phi)/\sqrt{2\pi}$ and $\hat{\rho}|\rho\rangle = \rho|\rho\rangle$, we find that

$$\psi_{nm}(\rho) = \sqrt{\frac{(n-m-1)!(2n-2)!}{(n+m-1)!}}\langle\rho|n, n-1\rangle\left[\frac{\left(n-\frac{1}{2}\right)a_0}{2\rho}\right]^{n-m-1} L_{n-m-1}^{2m}\left(\frac{2\rho}{\left(n-\frac{1}{2}\right)a_0}\right). \tag{149}$$

This leaves us with the task of computing the wavefunction for maximal m with a given n, that is, with $m = n-1$.

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Here is where we need to use the translation operator in polar coordinates. We derived the translation operator when acting on the $\langle 0_{\vec{\rho}}|$ bra in Eq. (76). Hence, we have that

$$\phi_n(\rho) = \langle \rho | n, n-1\rangle = \langle 0_\rho | \exp\left[\frac{i}{\hbar}\rho\left(\hat{p}_\rho + \frac{i\hbar}{2\hat{\rho}}\right)\right]|n, n-1\rangle. \tag{150}$$

As mentioned before, the best way to evaluate this expression is to find the eigenvector of $\left(\hat{p}_\rho + \frac{i\hbar}{2\hat{\rho}}\right)$. Using Eq. (137), we see that

$$\hat{p}_\rho \frac{1}{\hat{\rho}^{n-1}}|n, n-1\rangle = i\hbar\left[\frac{1}{\left(n-\frac{1}{2}\right)a_0} - \frac{1}{2\hat{\rho}}\right]\frac{1}{\hat{\rho}^{n-1}}|n, n-1\rangle, \tag{151}$$

which leads to the eigenvalue/eigenvector relationship

$$\left(\hat{p}_\rho + \frac{i\hbar}{2\hat{\rho}}\right)\frac{1}{\hat{\rho}^{n-1}}|n, n-1\rangle = \frac{i\hbar}{\left(n-\frac{1}{2}\right)a_0}\frac{1}{\hat{\rho}^{n-1}}|n, n-1\rangle. \tag{152}$$

Hence, we have that

$$\phi_n(\rho) = \langle 0_\rho | \frac{1}{\hat{\rho}^{n-1}}|n, n-1\rangle \rho^{n-1} \exp\left[-\frac{\rho}{\left(n-\frac{1}{2}\right)a_0}\right]. \tag{153}$$

Normalizing gives us

$$\langle 0_\rho | \frac{1}{\hat{\rho}^{n-1}}|n, n-1\rangle = \left[\frac{2}{\left(n-\frac{1}{2}\right)a_0}\right]^n \frac{1}{\sqrt{(2n-1)!}}. \tag{154}$$

Summarizing, we find that the normalized wavefunction is

$$\psi_{nm}(\rho, \phi) = \left[\frac{2}{\left(n-\frac{1}{2}\right)a_0}\right]^{|m|+1} \sqrt{\frac{(n-|m|-1)!}{(2n-1)(n+|m|-1)!}}\, \rho^{|m|} \exp\left[-\frac{\rho}{\left(n-\frac{1}{2}\right)a_0}\right] L^{2|m|}_{n-|m|-1}\left(\frac{2\rho}{\left(n-\frac{1}{2}\right)a_0}\right)\frac{e^{im\phi}}{\sqrt{2\pi}}. \tag{155}$$

This completes the calculation of the wavefunctions of the two-dimensional Coulomb problem.

IV. CONCLUSIONS

In this paper, we have shown how one can calculate wavefunctions in a representation-independent manner. The strategy starts from the origin in position space, translates to the position $\vec{r}$, and then computes the inner product with the energy eigenstate. Doing this for some central-potential problems requires us to convert the translation operator from Cartesian coordinates to spherical or polar coordinates because a Taylor series expansion for the wavefunctions of some problems does not exist in terms of the Cartesian coordinates. (This is true, for example, in the Coulomb problem but is not true for the two- or three-dimensional simple harmonic oscillator.) We illustrated how to convert from Cartesian coordinates to spherical (or polar) coordinates and then illustrated how the operator expression simplifies when it acts on the position-space eigenvector at the origin. Finally, we showed how such a procedure works by solving for the wavefunctions of the Coulomb problem in three and two dimensions. To do this requires us to use Schrödinger's factorization method, but we do so at the operator level only and do not convert the operators into the position-space representation. We want to emphasize that performing calculations in a representation-independent fashion illustrates that essentially all quantum properties are derived from the existence of a few eigenvectors (such as the position-space eigenvector at the origin and the ground-state eigenvector of the Coulomb problems) and the canonical commutation relations, $[\hat{r}_\alpha, \hat{p}_\beta] = i\hbar\delta_{\alpha\beta}$. No other assumptions are needed. This methodology is quite general, but it is simpler for position-space wavefunctions than for momentum-space wavefunctions. This is because the generic factorization method has raising and lowering operators that are linear in momentum operators but often are nonlinear in the position operators. Hence, it is easier to determine how the momentum operator acts on an energy eigenstate than to determine how a position operator acts. Nevertheless, this approach can be used in both position and momentum space and explicitly shows that these two wavefunctions are constructed in similar ways. The approach to determine them from "differential equations" is often quite different as the general formulation in momentum space is an integral equation rather than a differential equation, which is what is used in position space. This is true even though the two wavefunctions are directly related to each other via a Fourier transformation.

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APPENDIX: REPRESENTATION-INDEPENDENT CALCULATION OF COMMUTATORS

In the early years of quantum mechanics, Pauli[9] and Dirac[10] showed how to use the canonical commutation relation to compute commutators of functions of $\hat{r}_\alpha$ and $\hat{p}_\alpha$. We use the same method to compute the commutators needed in this work. To start, we compute the commutator of momentum with $\hat{r}^2 = \hat{r}_x^2 + \hat{r}_y^2 + \hat{r}_z^2$. Using the Leibniz rule for the commutator of a product, we immediately find that

$$\left[\hat{p}_\alpha, \hat{r}^2\right] = \hat{r}_\alpha[\hat{p}_\alpha, \hat{r}_\alpha] + [\hat{p}_\alpha, \hat{r}_\alpha]\hat{r}_\alpha = -2i\hbar\hat{r}_\alpha. \tag{A1}$$

Note that we never use the Einstein summation convention in this paper. Similarly, defining $\hat{r} = \sqrt{\hat{r}_x^2 + \hat{r}_y^2 + \hat{r}_z^2}$, the Leibniz rule shows that

$$\left[\hat{p}_\alpha, \hat{r}^2\right] = \hat{r}[\hat{p}_\alpha, \hat{r}] + [\hat{p}_\alpha, \hat{r}]\hat{r} = -2i\hbar\hat{r}_\alpha \tag{A2}$$

after using the result in Eq. (A1). The commutator $[\hat{p}_\alpha, \hat{r}]$ commutes with $\hat{r}$ as described by Böhm,[4] which follows from the triple commutator with $\hat{r}^2$,

$$\left[\hat{r}^2, [\hat{p}_\alpha, \hat{r}]\right] = \hat{r}[\hat{r}, [\hat{p}_\alpha, \hat{r}]] + [\hat{r}, [\hat{p}_\alpha, \hat{r}]]\hat{r}, \tag{A3}$$

and moving the $\hat{r}$ operator into the second element of the outermost commutator to multiply the term $[\hat{p}_\alpha, \hat{r}]$ for both nested commutators (which is valid because $[\hat{r}, \hat{r}] = 0$) yields

$$[\hat{r}, \hat{r}[\hat{p}_\alpha, \hat{r}] + [\hat{p}_\alpha, \hat{r}]\hat{r}] = \left[\hat{r}, \left[\hat{p}_\alpha, \hat{r}^2\right]\right] = [\hat{r}, (-2i\hbar\hat{r}_\alpha)] = 0 \tag{A4}$$

after substituting Eq. (A1) into the innermost commutator. Because the square root of an operator is uniquely defined to have the same eigenvectors as the original operator (but all eigenvalues are equal to the positive square roots of the eigenvalues of the original operators), if an operator $\hat{A}$ commutes with another operator $\hat{B}$, then the square root of $\hat{A}$ also commutes with $\hat{B}$. Hence, from Eq. (A4), we have $[\hat{r}, [\hat{p}_\alpha, \hat{r}]] = 0$. Combining this with Eq. (A2) gives us

$$[\hat{p}_\alpha, \hat{r}] = -i\hbar\frac{\hat{r}_\alpha}{\hat{r}}. \tag{A5}$$

One uses the Leibniz rule again to compute the commutator with $1/\hat{r}$ via

$$0 = [\hat{p}_\alpha, 1] = \left[\hat{p}_\alpha, \frac{\hat{r}}{\hat{r}}\right] = -i\hbar\frac{\hat{r}_\alpha}{\hat{r}^2} + \hat{r}\left[\hat{p}_\alpha, \frac{1}{\hat{r}}\right], \tag{A6}$$

which can be re-arranged to give

$$\left[\hat{p}_\alpha, \frac{1}{\hat{r}}\right] = i\hbar\frac{\hat{r}_\alpha}{\hat{r}^3}. \tag{A7}$$

Similarly, using $\hat{\rho} = \sqrt{\hat{r}_x^2 + \hat{r}_y^2}$, we find that $[\hat{p}_\alpha, \hat{\rho}] = -i\hbar\hat{r}_\alpha/\hat{\rho}$ for $\alpha = x$ or y and it vanishes for $\alpha = z$. We also find that $[\hat{p}_\alpha, 1/\hat{\rho}] = i\hbar\hat{r}_\alpha/\hat{\rho}^3$ with the same conditions on α.

Similarly, we define $\cos\hat{\theta} = \hat{r}_z/\hat{r}$, $\sin\hat{\theta} = \hat{\rho}/\hat{r}$, $\cos\hat{\phi} = \hat{r}_x/\hat{\rho}$, and $\sin\hat{\phi} = \hat{r}_y/\hat{\rho}$. Then, using the Leibniz rule, we find that

$$\left[\hat{p}_x, \cos\hat{\theta}\right] = i\hbar\frac{\hat{r}_x\hat{r}_z}{\hat{r}^3}, \quad \left[\hat{p}_y, \cos\hat{\theta}\right] = i\hbar\frac{\hat{r}_y\hat{r}_z}{\hat{r}^3}, \quad \left[\hat{p}_z, \cos\hat{\theta}\right] = -i\hbar\frac{\hat{\rho}^2}{\hat{r}^3}, \tag{A8}$$

$$\left[\hat{p}_x, \sin\hat{\theta}\right] = -i\hbar\frac{\hat{r}_x\hat{r}_z^2}{\hat{\rho}\hat{r}^3}, \quad \left[\hat{p}_y, \sin\hat{\theta}\right] = -i\hbar\frac{\hat{r}_y\hat{r}_z^2}{\hat{\rho}\hat{r}^3}, \quad \left[\hat{p}_z, \sin\hat{\theta}\right] = i\hbar\frac{\hat{\rho}\hat{r}_z}{\hat{r}^3}, \tag{A9}$$

$$\left[\hat{p}_x, \cos\hat{\phi}\right] = -i\hbar\frac{\hat{r}_y^2}{\hat{\rho}^3}, \quad \left[\hat{p}_y, \cos\hat{\phi}\right] = i\hbar\frac{\hat{r}_x\hat{r}_y}{\hat{\rho}^3}, \quad \left[\hat{p}_z, \cos\hat{\phi}\right] = 0, \tag{A10}$$

and

$$\left[\hat{p}_x, \sin\hat{\phi}\right] = i\hbar\frac{\hat{r}_x\hat{r}_y}{\hat{\rho}^3}, \quad \left[\hat{p}_y, \sin\hat{\phi}\right] = -i\hbar\frac{\hat{r}_x^2}{\hat{\rho}^3}, \quad \left[\hat{p}_z, \sin\hat{\phi}\right] = 0. \tag{A11}$$

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Of course, these "trigonometric function" operators commute with themselves and with $\hat{\rho}$ and $\hat{r}$ because all position operators commute with each other. Note that the angle operators are well defined *only* when they are arguments of the trigonometric functions. We never work with angle operators by themselves.

As described in the main text, we use the unit-vector operators ($\hat{\vec{e}}_r = \sin\hat{\theta}\cos\hat{\phi}\vec{e}_x + \sin\hat{\theta}\sin\hat{\phi}\vec{e}_y + \cos\hat{\theta}\vec{e}_z$, $\hat{\vec{e}}_\theta = \cos\hat{\theta}\cos\hat{\phi}\vec{e}_x + \cos\hat{\theta}\sin\hat{\phi}\vec{e}_y - \sin\hat{\theta}\vec{e}_z$, and $\hat{\vec{e}}_\phi = -\sin\hat{\phi}\vec{e}_x + \cos\hat{\phi}\vec{e}_y$) to define the components of momentum in spherical coordinates; in spherical coordinates, the unit vectors must be operators, while in Cartesian space, they are not. Using the symmetric combination of the dot product of momentum with these unit vectors (given schematically as $\frac{1}{2}\hat{\vec{e}}\cdot\hat{\vec{p}} + \frac{1}{2}\hat{\vec{p}}\cdot\hat{\vec{e}}$) and after computing the "quantum corrections" (proportional to $i\hbar$), we find that

$$\hat{p}_r = \sin\hat{\theta}\cos\hat{\phi}\hat{p}_x + \sin\hat{\theta}\sin\hat{\phi}\hat{p}_x + \cos\hat{\theta}\hat{p}_z - \frac{i\hbar}{\hat{r}}, \tag{A12}$$

$$\hat{p}_\theta = \cos\hat{\theta}\cos\hat{\phi}\hat{p}_x + \cos\hat{\theta}\sin\hat{\phi}\hat{p}_y - \sin\hat{\theta}\hat{p}_z - i\hbar\frac{\cot\hat{\theta}}{2\hat{r}}, \tag{A13}$$

and

$$\hat{p}_\phi = -\sin\hat{\phi}\hat{p}_x + \cos\hat{\phi}\hat{p}_y. \tag{A14}$$

Note that $\hat{p}_\phi$ does not have a quantum correction due to reordering. This is because it is equal to $\hat{L}_z/\hat{\rho}$.

Now that we have the components of momentum along the different spherical coordinate directions, we can use the commutation relations of the Cartesian components of momentum with the radial and angular operators to find that

$$[\hat{p}_r, \hat{r}] = -i\hbar, \quad [\hat{p}_r, \hat{\rho}] = -i\hbar\,\sin\hat{\theta} \tag{A15}$$

and the commutator of $\hat{p}_r$ with any trigonometric function of angles $\hat{\theta}$ and $\hat{\phi}$ is zero. We also have that $\hat{p}_\theta$ commutes with functions of $\hat{r}$ and $\hat{\phi}$. However, we have

$$\left[\hat{p}_\theta, \cos\hat{\theta}\right] = i\hbar\frac{\sin\hat{\theta}}{\hat{r}} \quad \text{and} \quad \left[\hat{p}_\theta, \sin\hat{\theta}\right] = -i\hbar\frac{\cos\hat{\theta}}{\hat{r}}. \tag{A16}$$

In addition, we have

$$[\hat{p}_\theta, \hat{\rho}] = -i\hbar\,\cos\hat{\theta}. \tag{A17}$$

Finally, for $\hat{p}_\phi$, we find that it commutes with trigonometric functions of $\hat{\theta}$ and arbitrary functions of $\hat{r}$ and $\hat{\rho}$. We also find that

$$\left[\hat{p}_\phi, \cos\hat{\phi}\right] = i\hbar\frac{\sin\hat{\phi}}{\hat{\rho}} \quad \text{and} \quad \left[\hat{p}_\phi, \sin\hat{\phi}\right] = -i\hbar\frac{\cos\hat{\phi}}{\hat{\rho}}. \tag{A18}$$

Surprisingly, because the projections of the momentum operator onto non-Cartesian unit-vector operators are not canonical momenta, we need to compute their commutators, which do not vanish, in general. We find that

$$[\hat{p}_r, \hat{p}_\theta] = \frac{i\hbar}{\hat{r}}\hat{p}_\theta, \tag{A19}$$

$$\left[\hat{p}_r, \hat{p}_\phi\right] = \frac{i\hbar}{\hat{r}}\hat{p}_\phi, \tag{A20}$$

and

$$\left[\hat{p}_\theta, \hat{p}_\phi\right] = i\hbar\frac{\cot\hat{\theta}}{\hat{r}}\hat{p}_\phi. \tag{A21}$$

In two dimensions, there are only a few changes. We define $\hat{\vec{e}}_\rho = (\hat{r}_x\vec{e}_x + \hat{r}_y\vec{e}_y)/\hat{\rho}$ and $\hat{\vec{e}}_\phi = (-\hat{r}_y\vec{e}_x + \hat{r}_x\vec{e}_y)/\hat{\rho}$, the latter vector being the same as in three dimensions. Using the trigonometric operators, these become

$$\hat{p}_\rho = \cos\hat{\phi}\hat{p}_x + \sin\hat{\phi}\hat{p}_y - \frac{i\hbar}{2\hat{\rho}} \tag{A22}$$

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and

$$\hat{p}_\phi = -\sin\hat{\phi}\hat{p}_x + \cos\hat{\phi}\hat{p}_y \tag{A23}$$

after evaluating the quantum correction for the radial momentum operator. The commutators are similar, and we report them here: first, for the radial momentum, which satisfies

$$[\hat{p}_\rho, \hat{\rho}] = -i\hbar, \tag{A24}$$

while $\hat{p}_\rho$ commutes with $\cos\hat{\phi}$ and $\sin\hat{\phi}$, and next, for the ϕ-component of the momentum

$$[\hat{p}_\phi, \cos\hat{\phi}] = i\hbar\frac{\sin\hat{\phi}}{\hat{\rho}} \quad \text{and} \quad [\hat{p}_\phi, \sin\hat{\phi}] = -i\hbar\frac{\cos\hat{\phi}}{\hat{\rho}}. \tag{A25}$$

We also have $[\hat{p}_\phi, \hat{\rho}] = 0$. Finally, we compute the commutation relation between the components of the momentum operator. This yields

$$[\hat{p}_\rho, \hat{p}_\phi] = \frac{i\hbar}{\hat{\rho}}\hat{p}_\phi. \tag{A26}$$

The last set of identities we derive in this appendix is the conversion of the kinetic-energy operator into its radial and angular components. Beginning in three dimensions, we find that

$$\begin{aligned}\hat{p}_r^2 &= \frac{1}{\hat{r}}(\hat{r}_x\hat{p}_x + \hat{r}_y\hat{p}_y + \hat{r}_z\hat{p}_z - i\hbar)\frac{1}{\hat{r}}(\hat{r}_x\hat{p}_x + \hat{r}_y\hat{p}_y + \hat{r}_z\hat{p}_z - i\hbar)\\ &= \frac{1}{\hat{r}^2}\left[\hat{r}_x^2\hat{p}_x^2 + \hat{r}_y^2\hat{p}_y^2 + \hat{r}_z^2\hat{p}_z^2 + 2\hat{r}_x\hat{r}_y\hat{p}_x\hat{p}_y + 2\hat{r}_y\hat{r}_z\hat{p}_y\hat{p}_z + 2\hat{r}_z\hat{r}_x\hat{p}_x\hat{p}_x - 2i\hbar(\hat{r}_x\hat{p}_x + \hat{r}_y\hat{p}_y + \hat{r}_z\hat{p}_z)\right].\end{aligned} \tag{A27}$$

Next, using the standard definition of orbital angular momentum,

$$\hat{L}_\alpha = \sum_{\beta\gamma}\epsilon_{\alpha\beta\gamma}\hat{r}_\beta\hat{p}_\gamma, \tag{A28}$$

we find that

$$\begin{aligned}\frac{\hat{\vec{L}}\cdot\hat{\vec{L}}}{\hat{r}^2} &= \frac{1}{\hat{r}^2}\left[(\hat{r}_x\hat{p}_y - \hat{r}_y\hat{p}_x)(\hat{r}_x\hat{p}_y - \hat{r}_y\hat{p}_x) + (\hat{r}_y\hat{p}_z - \hat{r}_z\hat{p}_y)(\hat{r}_y\hat{p}_z - \hat{r}_z\hat{p}_y) + (\hat{r}_z\hat{p}_x - \hat{r}_x\hat{p}_z)(\hat{r}_z\hat{p}_x - \hat{r}_x\hat{p}_z)\right]\\ &= \frac{1}{\hat{r}^2}\left[(\hat{r}_y^2 + \hat{r}_z^2)\hat{p}_x^2 + (\hat{r}_x^2 + \hat{r}_z^2)\hat{p}_y^2 + (\hat{r}_x^2 + \hat{r}_y^2)\hat{p}_z^2 - 2\hat{r}_x\hat{r}_y\hat{p}_x\hat{p}_y - 2\hat{r}_y\hat{r}_z\hat{p}_y\hat{p}_z - 2\hat{r}_z\hat{r}_x\hat{p}_x\hat{p}_x + 2i\hbar(\hat{r}_x\hat{p}_x + \hat{r}_y\hat{p}_y + \hat{r}_z\hat{p}_z)\right].\end{aligned} \tag{A29}$$

Adding together our results for $\hat{p}_r^2$ and $\vec{L}\cdot\vec{L}/\hat{r}^2$ yields

$$\frac{1}{2\mu}(\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2) = \frac{1}{2\mu}\left(\hat{p}_r^2 + \frac{\hat{\vec{L}}\cdot\hat{\vec{L}}}{\hat{r}^2}\right). \tag{A30}$$

Note that there are no quantum corrections in this case.

In two dimensions, we find that

$$\begin{aligned}\hat{p}_\rho^2 &= \frac{1}{\hat{\rho}}(\hat{r}_x\hat{p}_x + \hat{r}_y\hat{p}_y - \frac{i}{2}\hbar)\frac{1}{\hat{\rho}}(\hat{r}_x\hat{p}_x + \hat{r}_y\hat{p}_y - \frac{i}{2}\hbar)\\ &= \frac{1}{\hat{\rho}^2}\left[\hat{r}_x^2\hat{p}_x^2 + \hat{r}_y^2\hat{p}_y^2 + 2\hat{r}_x\hat{r}_y\hat{p}_x\hat{p}_y - i\hbar(\hat{r}_x\hat{p}_x + \hat{r}_y\hat{p}_y) + \frac{\hbar^2}{4}\right]\end{aligned} \tag{A31}$$

and

$$\frac{\hat{L}_z^2}{\hat{\rho}^2} = \frac{1}{\hat{\rho}^2}\left[\hat{r}_y^2\hat{p}_x^2 + \hat{r}_x^2\hat{p}_y^2 - 2\hat{r}_x\hat{r}_y\hat{p}_x\hat{p}_y + i\hbar(\hat{r}_x\hat{p}_x + \hat{r}_y\hat{p}_y)\right]. \tag{A32}$$

Again, adding these two together yields

$$\frac{1}{2\mu}(\hat{p}_x^2 + \hat{p}_y^2) = \frac{1}{2\mu}\left(\hat{p}_\rho^2 + \frac{\hat{L}_z^2 - \frac{1}{4}\hbar^2}{\hat{\rho}^2}\right). \tag{A33}$$

In this case, there is a quantum correction (namely, the term proportional to $\hbar^2$).

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DATA AVAILABILITY

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

REFERENCES

[1] E. Schrödinger, "A method of determining quantum-mechanical eigenvalues and eigenfunctions," Proc. R. Ir. Acad., Sect. A **46**, 9–16 (1940), available at https://www.jstor.org/stable/20490744.
[2] H. S. Green, *Matrix Mechanics* (P. Noordhoff, Ltd., Groningen, The Netherlands, 1965).
[3] H. C. Ohanian, *Principles of Quantum Mechanics* (Prentice-Hall, Inc., Englewood Cliffs, NJ, 1990).
[4] A. Böhm, *Quantum Mechanics Foundations and Applications*, 3rd ed. (Springer-Verlag, Inc., New York, 1993).
[5] E. Merzbacher, *Quantum Mechanics*, 3rd ed. (John Wiley & Sons, Inc., New York, 1998).
[6] P. Carruthers and M. M. Nieto, "Phase and angle variables in quantum mechanics," Rev. Mod. Phys. **40**, 411–440 (1968).
[7] M. Weitzman and J. K. Freericks, "Calculating spherical harmonics without derivatives," Condens. Matter Phys. **21**, 33002 (2018).
[8] J. L. Powell and B. Crasemann, *Quantum Mechanics* (Addison-Wesley, Reading, MA, 1961).
[9] W. Pauli, "On the hydrogen spectrum from the standpoint of the new quantum mechanics," Z. Phys. **36**, 336–363 (1926).
[10] P. A. M. Dirac, "The elimination of the nodes in quantum mechanics," Proc. R. Soc. London, Ser. A **111**, 281–305 (1926).

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