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Set of Generalized Uncertainty Relations and the Nature of the Uncertainty Principle

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A set of generalized uncertainty relations is derived for periodic systems. In the appropriate limits, they reduce to results previously obtained. The uncertainty principle is seen to express a relationship between the Fourier components of the wave function, ψ, and those of the probability density, $|\psi|^2$.

THE Heisenberg uncertainty relations are of great value in quantum mechanics, but there are difficulties associated with their applications to periodic functions. These difficulties have been overcome in principle during the past few years,[1] but the recent results are still unnecessarily restrictive. We have constructed a system of generalized uncertainty relations which appear to be quite useful, and which also shed some light on the basic nature of the uncertainty principle.

We consider the space of periodic functions such that $\psi(q+L)=\psi(q)$. For $L=2\pi$, this would include the single-valued functions of an angle variable, but the same formalism can also be used to describe a particle in a box with periodic boundary conditions. In either case, the conjugate momentum operator, $p=-i\partial/\partial q$, satisfies the commutation relation $[p,q]=-i$ and has a discrete spectrum. Since the periodicity condition requires that the eigenvalues of p satisfy $e^{ipL}=1$, these values must be integral multiples of $2\pi/L\equiv\lambda$.

The functions $\sin n\lambda q$ and $\cos n\lambda q$ are Hermitian operators on the function space and satisfy the commutation relations

$$[p,\,\sin n\lambda q]=-in\lambda\,\cos n\lambda q\,,$$
$$[p,\,\cos n\lambda q]=+in\lambda\,\sin n\lambda q\,.$$

We can therefore construct the uncertainty relations[2]

$$\Delta p\Delta\,\sin n\lambda q\geq\tfrac{1}{2}n\lambda\langle\cos n\lambda q\rangle\,,$$
$$\Delta p\Delta\,\cos n\lambda q\geq\tfrac{1}{2}n\lambda\langle\sin n\lambda q\rangle\,,$$

where $(\Delta p)^2=\langle p^2\rangle-\langle p\rangle^2$, etc. These relations are fairly straightforward generalizations of those obtained by Carruthers and Nieto.[1]

The nature of these inequalities is clarified if we use the trigonometric identities

$$\sin^2 n\lambda q=\tfrac{1}{2}(1-\cos 2n\lambda q)\,,$$
$$\cos^2 n\lambda q=\tfrac{1}{2}(1+\cos 2n\lambda q)$$

to evaluate $\Delta\,\sin n\lambda q$ and $\Delta\,\cos n\lambda q$. We obtain

$$(\Delta\,\sin n\lambda q)^2=\tfrac{1}{2}-\tfrac{1}{2}\langle\cos 2n\lambda q\rangle-\langle\sin n\lambda q\rangle^2\,,$$
$$(\Delta\,\cos n\lambda q)^2=\tfrac{1}{2}+\tfrac{1}{2}\langle\cos 2n\lambda q\rangle-\langle\cos n\lambda q\rangle^2\,.$$

The advantage of doing this is that the expectation values appearing in the uncertainty relations can all be expressed in terms of Fourier components of the particle density, which are

$$S_n=\langle\sin n\lambda q\rangle\,,\quad C_n=\langle\cos n\lambda q\rangle\,.$$

The result is

$$(\Delta p)^2(1-C_{2n}-2S_n^2)\geq\tfrac{1}{2}(n\lambda)^2C_n^2\,,\qquad\text{(UR1)}$$
$$(\Delta p)^2(1+C_{2n}-2C_n^2)\geq\tfrac{1}{2}(n\lambda)^2S_n^2\,.\qquad\text{(UR2)}$$

We can also combine these to form one somewhat simpler relation,

$$(\Delta p)^2(1-S_n^2-C_n^2)\geq(\tfrac{1}{2}n\lambda)^2(C_n^2+S_n^2)\,.\qquad\text{(UR3)}$$

This latter expression has the advantage of being invariant under translations, although clearly (UR3) does not contain as much information as (UR1) and (UR2) together do. The translational invariance of (UR3) is most easily seen by defining $\epsilon_n=C_n+iS_n=\langle e^{in\lambda q}\rangle$. As $C_n^2+S_n^2=|\epsilon_n|^2$, (UR3) reduces to the equivalent expression

$$\Delta p\geq\tfrac{1}{2}n\lambda|\epsilon_n|(1-|\epsilon_n|^2)^{-1/2}\,.\qquad\text{(UR3')}$$

[1] P. Carruthers and M. M. Nieto, Phys. Rev. Letters **14**, 387 (1965); Rev. Mod. Phys. **40**, 411 (1968).

[2] E. Merzbacher, *Quantum Mechanics* (Wiley, New York, 1970), pp. 158–160.

Since this relation depends only on the magnitude of ϵ_n, it is clearly invariant under translation. Further simplification of (UR1) and (UR2) is possible through a simple transformation of coordinates. We can define at least one point (to within $\frac{1}{2}L$ times an integer) q_n by $\langle \sin n\lambda(q-q_n)\rangle=0$. Under the coordinate change $q'=q-q_n$, where $S_n'=0$, (UR1) reduces to

$$\Delta p\Delta \sin n\lambda(q-q_n)=\Delta p(\tfrac{1}{2}-\tfrac{1}{2}C_{2n}')^{1/2}\geq\tfrac{1}{2}n\lambda C_n', \quad \text{(UR1}'\text{)}$$

while (UR2) gives the trivial result $\Delta p\geq 0$. The following examples will show that in various cases these can all be useful forms of the basic set of uncertainty relations, (UR1) and (UR2).

Derivation of the usual Heisenberg uncertainty relation is straightforward—we shall use (UR3′) to derive it. Explicit calculation of ϵ_n gives

$$\begin{aligned}\epsilon_n=\langle e^{in\lambda q}\rangle&=\int_{-L/2}^{L/2} e^{in\lambda q}|\psi|^2dq\\ &\simeq\int_{-L/2}^{L/2}(1+in\lambda q-\tfrac{1}{2}n^2\lambda^2q^2+\cdots)|\psi|^2dq\\ &=1+in\lambda\langle\langle q\rangle\rangle-\tfrac{1}{2}n^2\lambda^2\langle\langle q^2\rangle\rangle+\cdots,\end{aligned}$$

where we assume that $\psi(q)$ vanishes unless $|n\lambda q|\ll 1$ ($|nq|\ll L$), and $\langle\langle q^m\rangle\rangle$ refers to the local average of q^m as defined by the above integral; the point of this distinction is that because of the periodicity condition, $\psi(q+L)=\psi(q)$, $\langle q\rangle$ is undefined, which is the reason for this entire exercise (obviously $\langle e^{in\lambda q}\rangle$ and $\langle\langle e^{in\lambda q}\rangle\rangle$ are identical). So we get

$$\begin{aligned}|\epsilon_n|^2&\approx 1-n^2\lambda^2(\langle\langle q^2\rangle\rangle-\langle\langle q\rangle\rangle^2)+\cdots\\ &=1-n^2\lambda^2(\Delta q)^2+\cdots,\end{aligned}$$

where the above mathematical nicety is ignored in defining Δq, and substitution into (UR3′) gives

$$\Delta p\Delta q\geq\tfrac{1}{2}, \quad \text{(UR4)}$$

the factors of $n\lambda$ canceling out.

Let us now consider several examples in which both the usual uncertainty relation and the generalization of Carruthers and Nieto[1] give only the trivial result $\Delta p\geq 0$.

First, let $L=2\pi$ (e.g., q can be a physical angle) and let $\psi(q)=(\cos q)/\sqrt{\pi}$, so

$$\epsilon_n=\int_{-\pi}^{\pi} e^{inq}\cos^2q\,dq/\pi.$$

The only nonvanishing values (other than ϵ_0) are $\epsilon_{\pm 2}=\frac{1}{2}$, and (UR3′) gives $\Delta p\geq 1/\sqrt{3}$. This is not the strongest uncertainty relation we can obtain, however. For all n, $S_n=\langle\sin nq\rangle=0$, and except for $n=0$ the only nonzero value of C_n is $C_2=\frac{1}{2}$, so either (UR1) or (UR1′) gives $\Delta p\geq 1/\sqrt{2}$. The actual value of Δp is easily evaluated to be exactly 1.

Next, consider a sequence of uniform pulses a finite distance D apart, and let L be very large but finite (we can take the $L\to\infty$ limit later). The periodic boundary condition on ψ requires that $L=ND$, where N is an integer. All values of ϵ_n are zero until we get to

$$\begin{aligned}\epsilon_N=\langle e^{iN\lambda q}\rangle&=\langle e^{2\pi iq/D}\rangle\\ &=\int_{-L/2}^{L/2} e^{2\pi iq/D}|\psi|^2dq\\ &=N\int_{-D/2}^{D/2} e^{2\pi iq/D}|\psi|^2dq.\end{aligned}$$

If the pulses are well separated, so that $\psi(q)$ vanishes unless $|q|\ll D$, we can repeat the derivation of (UR4) and again we get $\Delta p\Delta q\geq\frac{1}{2}$, where Δq, the width of an individual pulse, is expressed in terms of local averages.

Of course, the pulses need not be so well separated for a useful uncertainty relation to exist. For example, a Bloch wave has the form $\psi(x)=e^{ikx}U(x)$, where $U(x+a)=U(x)$. This method enables us to describe the dispersion of the real momentum, which can be measured by means of positron annihilation, in terms of the Fourier components of $|U(x)|^2$. An interesting feature of this is that the wave function itself is not periodic (except in terms of the arbitrarily large distance L), but the uncertainty relation depends only on the probability density, and the momentum dispersion is determined by the localization of the electrons within the unit cell.

It appears that the above set of uncertainty relations will prove useful in situations where previous forms of these relations give only the trivial result $\Delta p\geq 0$. The form of the relations also sheds light on the nature of the uncertainty principle itself, which proves quite simply to relate the Fourier components of the wave functions, ψ, to the Fourier components of the probability density, $|\psi|^2$.