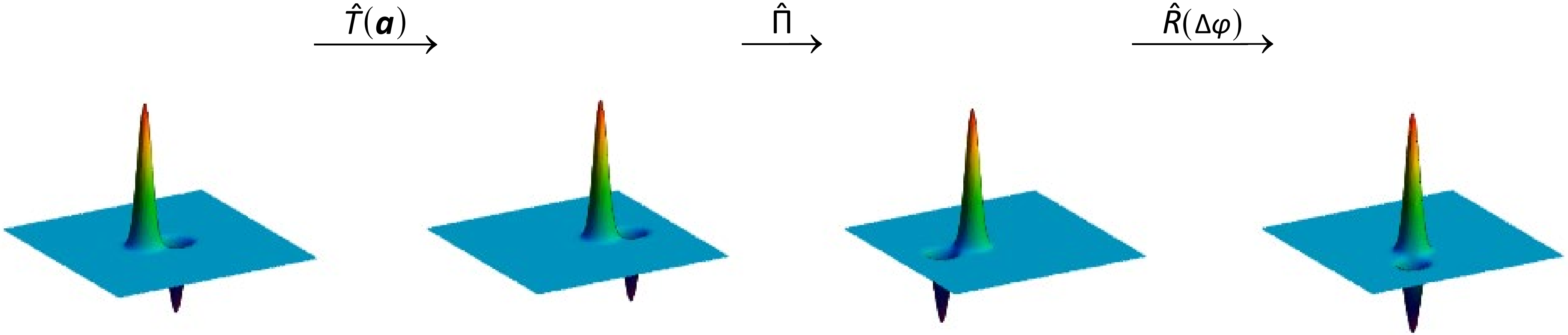
Today in Physics 237: transformations and symmetry

- Symmetry and transformation operators
- The translation operator
- Continuous translational symmetry: momentum conservation
- Discrete translational symmetry: Bloch’s theorem, crystals, energy bands and band gaps.



Logistical announcement

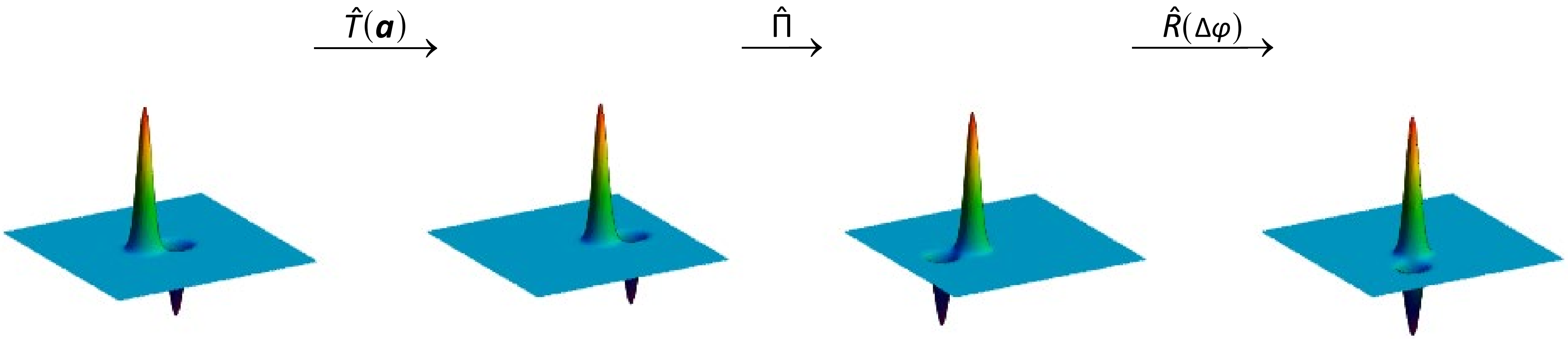
- I will be traveling for the rest of the week, leaving directly when we’re done today.
- Fortunately, **proto-Dr. Vedang Bhelande** is still here, and doesn’t have any class conflicts with this one
- On Thursday, 23 April 2026, Vedang will administer Quiz #12 as usual, and directly thereafter he will deliver Lecture #26, on Parity. Many thanks to Vedang
- I return to ROC about 4:30 on Friday, so consider Friday’s office hours cancelled this week.

Symmetry

- By **transformation**, we mean a mathematical change to the spacetime coordinates or other properties we use to define a physical system.
  - First example: **translation**. Replace x in a state vector, operator, or equation of motion with $x = x - a$.
- Transformation can be discrete or continuous.
  - Most transformations of use in classical physics are continuous, but of course in quantum mechanics we have plenty of opportunity to use discrete ones.
  - First examples: discrete translation, such as in a crystalline solid with atoms all the same distance a apart, or continuous translation, such as a continuously-variable parameter a.
- A transformation made to a state vector or operator, or to the Schrödinger equation, could change the system to something completely different. Most interesting are when these mathematical objects are **invariant** under the transformation.
  - Invariance under a transformation is what we mean by **symmetry**.

Transformation operators

- As we did for exchange of quanta in a two-quantum state function, we can define operators which carry out transformations, like
  - translation $\hat{T}(\boldsymbol{a})$: $\hat{T}(\boldsymbol{a})\psi(\boldsymbol{r}) = \psi'(\boldsymbol{r}) = \psi(\boldsymbol{r}-\boldsymbol{a})$
  - coordinate inversion $\hat{\Pi}$ – **parity**, closely related to the exchange operator $\hat{P}$ ([Lecture 23](#)): $\hat{\Pi}\psi(\boldsymbol{r}) = \psi'(\boldsymbol{r}) = \psi(-\boldsymbol{r})$
  - rotation ([Lecture 9](#)), for example about *z*: $\hat{R}(\Delta\varphi)\psi(\boldsymbol{r}) = \psi'(\boldsymbol{r}) = \psi(r,\vartheta,\varphi-\Delta\varphi)$



The translation operator

- Expand $\hat{T}(a)\psi(x)=\psi(x-a)$ in a Taylor series about x = 0, and recall $e^u=\sum_{n=0}^{\infty}\frac{u^n}{n!}$:

$$\hat{T}(a)\psi(x)=\psi(x-a)=\sum_{n=0}^{\infty}\frac{1}{n!}(-a)^n\frac{d^n}{dx^n}\psi(x)=\sum_{n=0}^{\infty}\frac{1}{n!}\left(-a\frac{1}{-i\hbar}\hat{p}\right)^n\psi(x)=e^{-ia\hat{p}/\hbar}\psi(x)\quad\Rightarrow\quad\boxed{\hat{T}(a)=e^{-ia\hat{p}/\hbar}}\quad .$$

  - In this form, the momentum operator $\hat{p}$ is the **generator** of the translation along *x.*

- See Lecture 12 for how to use exponentials of operators (basically, go back one step from this result), but the compact form is useful to show that $\hat{T}$ is a unitary transformation:

$$\hat{T}(-a)=\left(\hat{T}(a)\right)^{-1}=\left(\hat{T}(a)\right)^{*}=\left(\hat{T}(a)\right)^{\dagger}\quad ,$$

  and thus preserves the magnitudes of state vectors.

- $\hat{T}$ can translate operators as well as, or instead of, state vectors. For operator $\hat{Q}$, state ψ and translated state ψ',

$$\langle\psi'|\hat{Q}|\psi'\rangle=\langle\psi|\hat{T}(a)^{\dagger}\hat{Q}\hat{T}(a)|\psi\rangle=\langle\psi|\hat{Q}'|\psi\rangle\quad\Rightarrow\quad\boxed{\hat{Q}'=\hat{T}(a)^{\dagger}\hat{Q}\hat{T}(a)}\quad .$$

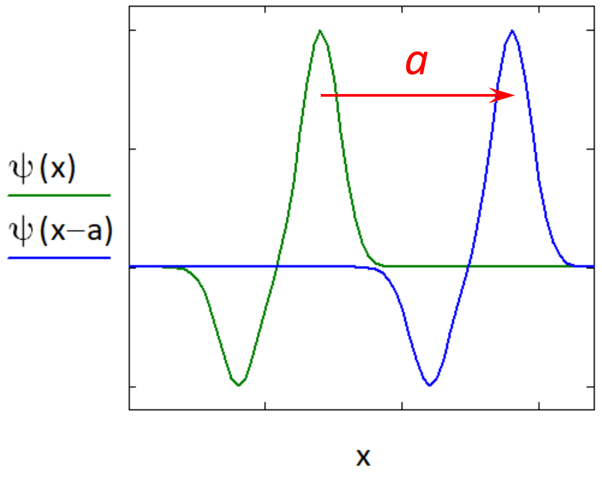
The translation operator (continued)

- Think of the difference between translating wavefunction and operator as follows:
  - $\hat{T}(a)|\psi(x)\rangle = |\psi(x-a)\rangle$ keeps the coordinate system the same and shifts each point in the wavefunction toward +*x*, by amount *a*.
  - Or one could shift the coordinate origin toward –*x*, by amount *a*. Then $\hat{Q}' = \hat{T}(a)^{\dagger}\hat{Q}\hat{T}(a)$ is the shifted-coordinate-system version of the operator.

Mathematically equivalent, of course.

- For example (G&S 6.1), let's translate $\hat{x}$ itself.
  - First: note that if $\psi(x)$ is an eigenstate of $\hat{x}$ with eigenvalue *x*, then $\psi(x-a)$ is an eigenstate of $\hat{x}$ with eigenvalue $x + a$.

    (The whole function is translated to the right; every value of ψ formerly at *x* is now at $x + a$. Potentially confusing.)



The translation operator (continued)

- Next a related, immediately useful, example: calculate $\left[\hat{x},\hat{T}\right]$.

$$\hat{T}(a)\hat{x}\left|\psi(x)\right\rangle = x\hat{T}(a)\left|\psi(x)\right\rangle = x\left|\psi(x-a)\right\rangle \quad ,$$

$$\hat{x}\hat{T}(a)\left|\psi(x)\right\rangle = \hat{x}\left|\psi(x-a)\right\rangle = (x+a)\left|\psi(x-a)\right\rangle \quad ;$$

$$\left[\hat{x},\hat{T}(a)\right]\left|\psi(x)\right\rangle = (x+a-x)\left|\psi(x-a)\right\rangle = a\hat{T}(a)\left|\psi(x)\right\rangle \quad \Rightarrow \quad \boxed{\left[\hat{x},\hat{T}(a)\right] = a\hat{T}(a)} \quad .$$

- Now: the translated version of $\hat{x}$ is, from page 4, $\hat{x}' = \hat{T}(a)^{\dagger}\hat{x}\hat{T}(a)$. Use the new commutator:

$$\hat{x}'\left|\psi(x)\right\rangle = \hat{T}(a)^{\dagger}\hat{x}\hat{T}(a)\left|\psi(x)\right\rangle = \hat{T}(a)^{\dagger}\left(\hat{T}(a)\hat{x} + a\hat{T}(a)\right)\left|\psi(x)\right\rangle$$

$$= \hat{T}(a)^{\dagger}\hat{T}(a)(\hat{x}+a)\left|\psi(x)\right\rangle = (\hat{x}+a)\left|\psi(x)\right\rangle \quad \Rightarrow \quad \boxed{\hat{x}' = \hat{x}+a} \quad .$$

1   $\hat{T}$ is unitary

The translation operator (continued)

- In G&S problems 6.3 and 6.4 on this week's assignment, you will show that the momentum operator $\hat{p}$ is invariant under translation:

$$\hat{p}' = \hat{T}(a)^\dagger \hat{p}\hat{T}(a) = \hat{p} \quad \ldots$$

  - Of course: momentum depends only on **differences** in position $\left(\text{i.e. } \hat{p} = m\,\mathbf{d\hat{x}}/dt\right)$.
  - Also harmonizes with momentum being the generator of $\hat{T}$.

- … and thus any operator $\hat{Q}$ behaves under translation according to

$$\boxed{\hat{Q}'(\hat{x},\hat{p}) = \hat{T}(a)^\dagger \hat{Q}(\hat{x},\hat{p})\hat{T}(a) = \hat{Q}(\hat{x}',\hat{p}') = \hat{Q}(\hat{x}+a,\hat{p}) \quad .}$$

See also Lecture 2, p. 12.

The translation operator (continued)

- We can calculate the eigenvalues of $\hat{T}(a)$ from its properties as a unitary transformation. Suppose that $|\psi\rangle$ is a normalized eigenstate of $\hat{T}(a)$, with eigenvalue λ; then

$$1 = \langle\psi|\psi\rangle = \langle\psi|\hat{T}(a)^\dagger \hat{T}(a)|\psi\rangle = \lambda^*\lambda\langle\psi|\psi\rangle = |\lambda|^2 \quad .$$

- Any complex number of magnitude 1 can be written as $\boxed{\lambda = e^{i\varphi},}$ where φ is a real number.

Translational symmetry

- Invariance means that an operator's expectation values are time-independent. According to the generalized Ehrenfest theorem (Lecture 11, p. 5) this would mean that the operator commutes with the Hamiltonian: $\left[\hat{H},\hat{Q}\right]=0$.
  - Also that it has no explicit time dependence: $\left\langle \partial\hat{Q}/\partial t\right\rangle = 0$.
- And indeed the translation operator meets both criteria: $\hat{H}'=\hat{T}^{\dagger}\hat{H}\hat{T}=\hat{H} \quad\Rightarrow\quad \hat{T}\hat{T}^{\dagger}\hat{H}\hat{T}=\hat{T}\hat{H} \quad\Rightarrow\quad \boxed{\left[\hat{H},\hat{T}\right]=0}$.
- So if, in 1-D, a single quantum is described by the usual Hamiltonian $\hat{H}=\hat{p}^2/2m+V(x)$, then translational invariance implies that the quantum is subjected to this potential:

$$V(x)=V'(x)=\hat{T}^{\dagger}V(x)\hat{T}=V(x')=\boxed{V(x+a)}\ .$$

- This outcome has two different implications in two different, interesting settings.
- If a is a **continuously-variable parameter**, then $V(x)=V(x+a)$ can only mean that ***V* is uniform**: a constant offset to the Hamiltonian.
  - This is the setup for a free-quantum wavepacket (Lectures 6, 7, 8, 11).

Translational symmetry (continued)

- And the setup has the same consequences in quantum mechanics as in classical mechanics: that **continuous translational symmetry = conservation of momentum**.
- In math and classical mechanics, this result stems from Noether's Theorem #1: ***if an equation of motion has a continuous symmetry, then there is a conserved quantity corresponding to the symmetry, and vice versa*** (Noether 1918).
- To prove Noether's theorem, one uses calculus of variations and Lagrangian expressions for the equations of motion, so we will hope you will see such a proof in PHYS 235.
- But we can easily **demonstrate** that continuous translational symmetry leads to momentum conservation, using the generating function (page 4): for $\delta \ll \hbar/p$ and to first order in δ,

$$\hat{T}(\delta) = e^{-i\delta\hat{p}/\hbar} \cong 1 - \frac{i\delta\hat{p}}{\hbar} \quad \Rightarrow \quad \left[\hat{H}, \hat{T}(\delta)\right] = \left[\hat{H}, 1 - \frac{i\delta\hat{p}}{\hbar}\right] = -\frac{i\delta}{\hbar}\left[\hat{H}, \hat{p}\right] = \frac{i\hbar\delta}{2m}\left[\hat{p}^2, \hat{p}\right] = 0 \quad \Rightarrow \quad \frac{d}{dt}\langle p \rangle = 0$$

, q.e.d.,

where Ehrenfest's theorem (Lecture 11, p. 5) is used in the last step.

Periodic potential energy: Bloch's theorem

- If a is a **discrete value** of distance, then $V(x) = V(x+a)$ is in general not uniform, but its values repeat with every – that is, V varies periodically with position, with period a – has no classical counterpart, but turns out to involve a wavepacket solution too:

  - Since $\left[\hat{H}, \hat{T}(a)\right] = 0$ is the condition under which $V(x) = V(x+a)$, the eigenstates of $\hat{H}$ and $\hat{T}(a)$ can be chosen to be the same.

    - That is: if a basis of eigenstates is chosen so that $\vec{H}$ only has nonzero elements along the diagonal, $\vec{T}(a)$ will also be diagonal.

  - Call the eigenstates $\psi(x)$ as usual, with $\hat{H}\psi(x) = E\psi(x)$ and $\hat{T}(a)\psi(x) = \lambda\psi(x) = e^{i\varphi}\psi(x)$.

  - Let $\varphi = -qa$. Because q has dimensions 1/distance = momentum/$\hbar$, $\hbar q$ is called the **crystal momentum**.

  - But $\hat{T}(a)$ is still the translation operator, so $\hat{T}(a)\psi(x) = e^{-iqa}\psi(x)$ and $= \psi(x-a)$ $\Rightarrow$ $\psi(x-a) = e^{-iqa}\psi(x)$.

  - Now define a new function $u(x)$ such that $\psi(x) = e^{iqx}u(x)$:

Periodic potential energy: Bloch's theorem (continued)

$$e^{iq(x-a)}u(x-a)=e^{-iqa}e^{iqx}u(x) \quad \Rightarrow \quad u(x-a)=u(x) \quad .$$

- And substitute back:

$$\boxed{\psi(x)=e^{iqx}u(x), \quad \text{with } u(x)=u(x-a) \quad .}$$

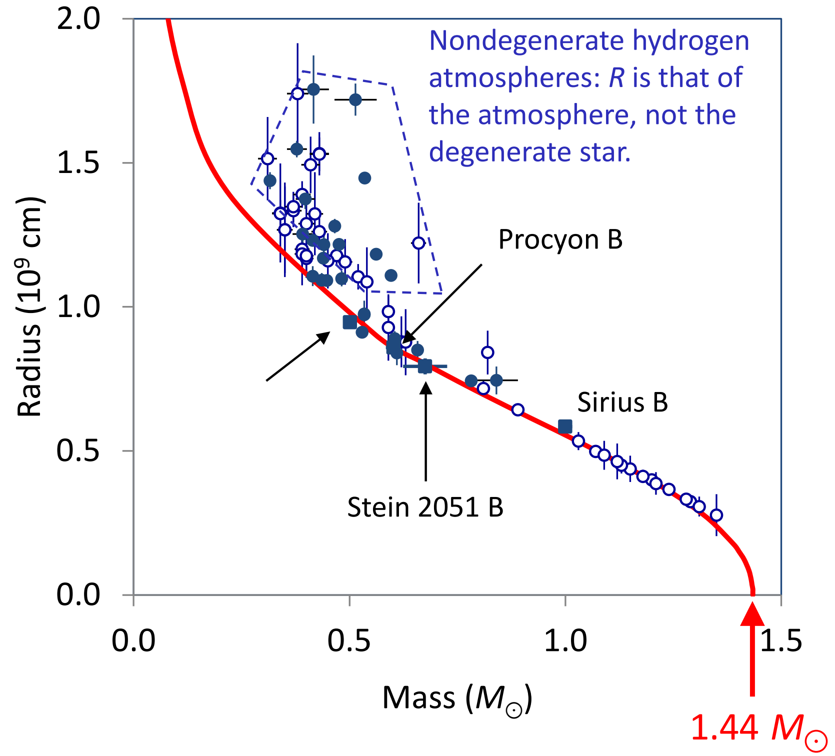
Bloch's theorem

- This all looks trivial and therefore not very important – I thought so too, the first time I saw it – so let's add some emphasis:
  - If one subjects a quantum to a spatially-periodic potential energy, one gets a wavefunction with a spatially-periodic factor.
  - And the spatially-periodic factor of the wavefunction comes with a travelling-wave factor: quanta moving through the medium which supplies the potential, at wave speed $v=\hbar q/2m$ which is independent of position in the medium.
  - One can think of the quanta as modulated travelling waves, delocalized from the sources of the potential energy, propagating without loss of energy and momentum from scattering.

Applications of the free electron gas and Bloch's theorem

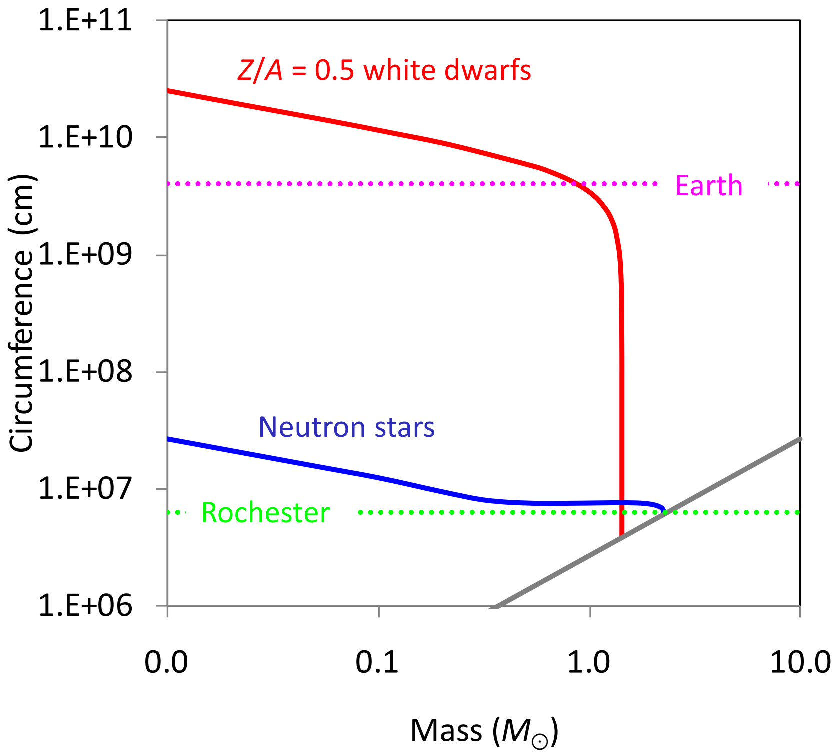
1. White dwarfs and neutron stars (see ASTR 241)

- At the end of a low-mass star's life, thermal pressure declines sharply: the star keeps shining but the luminosity is no longer replenished, due to exhaustion of nuclear-fusion fuel.
- The declining thermal pressure can no longer support the weight of the star, so over the course of a few Myr, it contracts to smaller size, heating up as it does so.
- Degeneracy pressure of electrons increases as the star contracts; the contraction stops when degeneracy pressure balances the weight.
- And if the star's mass $M < 1.44 M_\odot$ at this point, it will be in this state til the end of time: the electrons are degenerate; the population of atomic nuclei ("ions"), still behaving as an ideal gas with temperature T_0, continues to cool as time goes on.



Applications of the free electron gas and Bloch's theorem (continued)

- When the ion temperature T_0 drops below about 10^6 K, the ions – commonly, former nuclei of ^{12}C and ^{16}O – **crystallize**.
  - Thus moving from continuous translational invariance to discrete translational invariance, and the domain of Bloch's theorem.
- The end state is a Solar-mass weight, terrestrial-planet-size, ion crystal: its weight supported and ion-repulsion neutralized by electron degeneracy pressure, its electrons all delocalized.
- For dead stars with final masses $1.44M_{\odot} < M < 2.3M_{\odot}$, the end state is a terrestrial-city-size neutron-spin crystal, supported by neutron degeneracy pressure.



Applications of the free electron gas and Bloch's theorem (continued)

2. **Energy bands in crystalline solids** (see G&S section 5.3.2)

- In crystals – the best example of discrete translational invariance, quanta can indeed propagate freely through the medium loss of energy and momentum from scattering, but only at certain energies.

- This is an outcome of the modulation of the wavefunction by the periodically-varying potential energy:

  - Consider a crystal made of atoms, each of which has one electron which is delocalized, as described on p. 12.

  - The site of each atom is a potential well for the electrons.

  - Delocalized electrons, travelling through the crystal as wavepackets, can be transmitted or reflected (scattered, in 3-D) by the potential wells they encounter, as we discussed in Lectures 7 and 8.

  - Just as in the case of reflection from or tunneling through a potential well, as considered in Lecture 8 (esp. p. 22), **constructive or destructive interference** of the traveling waves will therefore occur, changing the waves' amplitudes by amounts determined by the size or spacing of the potential wells.

Applications of the free electron gas and Bloch's theorem (continued)

- Thus a crystal acts like a three-dimensional **diffraction grating** for the traveling waves of electrons.
- And just as is the case for light interacting with an optical diffraction grating (PHYS 143 experiments 13 and 14), constructive interference makes an electron energy E $\left(\text{for light, wavelength } \lambda = hc/E\right)$ match up only with certain electron momenta $\boldsymbol{p} = \hbar \boldsymbol{k}$ $\left(\text{for light, the angle } \vartheta\text{, which is the direction of the light's momentum}\right)$.
- This is what, for diffraction gratings, produces the different **orders** of interference, and the dispersion of wavelengths into different angles within an order.
- In the case of crystals, it leads to propagation of electrons through the crystal ***only with specific combinations of E and k.***
- G&S consider the example of a 1-D crystal of delta-function potentials, finding the energies at which quanta can propagate (**bands**) and those at which they cannot (**band gaps**):

$$\cos qa = \cos ka + \frac{m\alpha}{\hbar^2 k}\sin ka \quad ,$$

Compare to the grating equation

where $\hbar q$ is crystal momentum, $k = \sqrt{2mE}/\hbar$, and a and α the period and amplitude of the potential energy.

Applications of the free electron gas and Bloch's theorem (continued)

- G&S figure 5.5E, for bands and gaps in a 1-D crystal, compared to a reflection-mode diffraction grating.