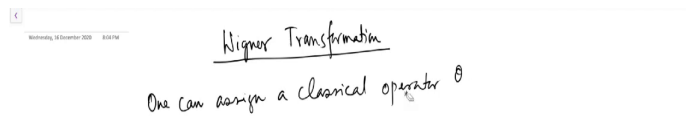


Statistical Mechanics
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Lecture - 46
Wigner Transformation

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So, now we look at what is called the Wigner Transformation. Some of you may already have learned this in quantum mechanics, but its very brief review that we do.

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One can assign a classical observable $O_{cl}(\vec{r}, \vec{p})$ corresponding to a quantum mechanical operator $\hat{O}(\vec{r}, \vec{p})$

$$O_{cl}(\vec{r}, \vec{p}) = \int \langle \vec{R} - \vec{r}/2 | \hat{O} | \vec{R} + \vec{r}/2 \rangle e^{i\vec{p} \cdot \vec{r}} d^3r$$

Quantization prescription by Heyl.

For every classical observable $O_{cl}(\vec{r}, \vec{p})$, the matrix representation of $\hat{O}(\vec{r}, \vec{p}) \equiv$



The idea is that one can assign a classical operator O or let us not call it classical operator, let us call it classical observable $O_{cl} r, p$ corresponding to a quantum mechanical operator $\hat{O} r, p$ right and the prescription to do that is $O_{cl} r, p$ is integral R minus r by 2 \hat{O} R plus r by 2 e to the power $i p \cdot r$ $d^3 r$, right.

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Niquist Transformation



One can assign a classical observable $O_{cl}(\vec{r}, \vec{p})$ corresponding to a quantum mechanical operator $\hat{O}(\vec{r}, \vec{p})$

$$O_{cl}(\vec{r}, \vec{p}) = \int \langle \vec{R} - \frac{\vec{r}}{2} | \hat{O} | \vec{R} + \frac{\vec{r}}{2} \rangle e^{i\vec{p} \cdot \vec{r}} d\vec{r}$$

$d\vec{p} = d^3p$

Quantization prescription by Weyl.

For every classical observable $O_{cl}(\vec{r}, \vec{p})$, the matrix representation of $\langle \vec{r}' | \hat{O} | \vec{r} \rangle$ in the coordinate representation

$$\langle \vec{r}' | \hat{O} | \vec{r} \rangle = \frac{1}{i^3} \int O_{cl} \left(\frac{\vec{r} + \vec{r}'}{2}, \vec{p} \right) e^{\frac{i}{\hbar} \vec{p} \cdot (\vec{r}' - \vec{r})} d\vec{p}$$



The inverse of this is the quantization prescription by Weyl and here, the idea is that for every classical observable $O_{cl}(\vec{r}, \vec{p})$, the matrix representation of $\hat{O}(\vec{r}, \vec{p})$ which is sorry we will say that the matrix representation of this since, we are saying the matrix representation, this becomes $\langle \vec{r}' | \hat{O} | \vec{r} \rangle$ of this quantum mechanical operator \hat{O} is given by so, this is in the coordinate representation.

So, in the coordinate representation is given by $\langle \vec{r}' | \hat{O} | \vec{r} \rangle = \frac{1}{i^3} \int O_{cl}(\frac{\vec{r} + \vec{r}'}{2}, \vec{p}) e^{\frac{i}{\hbar} \vec{p} \cdot (\vec{r}' - \vec{r})} d\vec{p}$. Now, the measure is different I have so, this is identical to d^3p where now \vec{p} is a scalar matrix and if you want to write down this, we can write down this as a vector \vec{r} , but essentially the idea is same right.

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$$\langle \hat{r}' | \hat{\rho} | r \rangle = \frac{1}{\lambda^3} \int d\vec{r} e^{-\pi i (\vec{r}' - \vec{r})^2 / \lambda^2}$$

$$\hat{O} \equiv \hat{\rho}$$

$$\langle \hat{r}' | \hat{\rho} | \hat{r} \rangle = \frac{1}{V} e^{-\pi (\vec{r}' - \vec{r})^2 / \lambda^2}$$

$$\langle \vec{R} - \frac{\vec{r}}{2} | \hat{\rho} | \vec{R} + \frac{\vec{r}}{2} \rangle = \frac{1}{V} e^{-\pi (\vec{R} - \frac{\vec{r}}{2} - \vec{R} - \frac{\vec{r}}{2})^2 / \lambda^2} = \frac{1}{V} e^{-\pi \vec{r}^2 / \lambda^2}$$

$$\rho(\vec{R}, \vec{p}) = \int d\vec{r} \frac{1}{V} e^{-\pi \vec{r}^2 / \lambda^2} e^{i \vec{p} \cdot \vec{r} / \hbar}$$



Let us see if we can first really validate this for a case of a single particle. So, let us take \hat{O} as identical to the density matrix in the canonical ensemble and there, we have $\langle \hat{r}' | \hat{\rho} | \hat{r} \rangle = \frac{1}{V} e^{-\pi (\vec{r}' - \vec{r})^2 / \lambda^2}$ was 1 by v e to the power minus pi r prime minus r whole square divided by lambda T square.

So, following the Wigner transformation, we write this as $\langle \vec{R} - \frac{\vec{r}}{2} | \hat{\rho} | \vec{R} + \frac{\vec{r}}{2} \rangle$ and this becomes $\frac{1}{V} e^{-\pi (\vec{R} - \frac{\vec{r}}{2} - \vec{R} - \frac{\vec{r}}{2})^2 / \lambda^2}$ which is $\frac{1}{V} e^{-\pi \vec{r}^2 / \lambda^2}$ square over lambda T square.

Therefore, the classical observable which is $\rho(\vec{R}, \vec{p})$ is the Wigner transformation tells me that corresponding to this quantum mechanical operator, there is a classical observable which we will call ρ of capital R comma p and that prescription is given by this so, we take it as

integral d of r 1 by v e to the power minus pi r square over lambda T square e to the power i p dot r.

This clearly is a Gaussian, there has to be a h bar over here. So, did I miss an h bar over here, there is a h bar over here. Now, this clearly is a Gaussian integral.

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$$\langle \vec{r} | \beta | r \rangle = \frac{1}{V}$$



$$\langle \vec{r} - \frac{\vec{r}}{2} | \frac{\vec{r}}{2} | \vec{r} + \frac{\vec{r}}{2} \rangle = \frac{1}{V} e^{-\pi (\vec{r} - \frac{\vec{r}}{2} - \vec{r} - \frac{\vec{r}}{2})^2 / \lambda^2} = \frac{1}{V} e^{-\pi r^2 / \lambda^2}$$

$$\psi(\vec{r}, \vec{p}) = \int d\vec{r} \frac{1}{V} e^{-\pi r^2 / \lambda^2} e^{i \vec{p} \cdot \vec{r} / \hbar}$$

$$e^{-\frac{\pi}{\lambda^2} (r^2 - i \frac{\vec{p} \cdot \vec{r}}{\hbar} \frac{\lambda^2}{\pi})}$$

$$r^2 - i \frac{\vec{p} \cdot \vec{r}}{\hbar} \frac{\lambda^2}{\pi} \equiv \left(\vec{r} - \frac{i \vec{p} \lambda^2}{2\pi \hbar} \right)^2$$

$$r^2 - i \frac{\vec{p} \cdot \vec{r}}{\hbar} \frac{\lambda^2}{\pi} + \left(\frac{i \lambda^2}{2\pi} \right)^2 \vec{p}^2$$

$$\left[r^2 - i \frac{\vec{p} \cdot \vec{r}}{\hbar} \frac{\lambda^2}{\pi} - \left(\frac{\lambda^2}{2\pi} \right)^2 \vec{p}^2 \right]$$



Then, this expression over here I can manipulate in the following way r square minus i p dot r lambda T square over pi is identical to r minus i p dot lambda T square times 2 pi whole square so that this gives me r square minus i p dot r lambda T square of a pi plus i lambda T square over 2 pi whole square p square which is now a scalar because p square is p dot p so, we will write this as p, but I clearly have this factor over here.

So, this is $r^2 - i \vec{p} \cdot \vec{r} \frac{\lambda T}{\pi} - \left(\frac{\lambda T}{2\pi}\right)^2 p^2$ over π minus λT square over 2π whole square p^2 , but I realize that there is a minus sign which is outside so, then the term that I need to add is plus so, this minus and this minus makes it a minus therefore, I need to add a term which is plus λT square over 2π whole square times p^2 .

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$$\begin{aligned}
 & \left[r^2 - i \vec{p} \cdot \vec{r} \frac{\lambda T}{\pi} - \left(\frac{\lambda T}{2\pi}\right)^2 p^2 \right] \\
 & e^{-\frac{\pi}{\lambda T^2} \left[r^2 - i \vec{p} \cdot \vec{r} \frac{\lambda T}{\pi} + \left(\frac{\lambda T}{2\pi}\right)^2 p^2 \right]} + \left(\frac{\lambda T}{2\pi}\right)^2 p^2 \\
 & e^{-\frac{\pi}{\lambda T^2} \left(r^2 - i \frac{\lambda T}{2\pi} \vec{p} \cdot \vec{r} \right)^2} - \frac{\pi}{\lambda T^2} \frac{\lambda T^2}{4\pi^2} p^2 \\
 & e^{-\frac{\pi}{\lambda T^2} \left(r^2 - i \frac{\lambda T}{2\pi} \vec{p} \cdot \vec{r} \right)^2} e^{-\frac{\lambda T^2}{4\pi^2} p^2} \\
 & e^{-\frac{\pi}{\lambda T^2} \left(r^2 - i \frac{\lambda T}{2\pi} \vec{p} \cdot \vec{r} \right)^2} e^{-\frac{\lambda T^2}{4\pi^2} p^2}
 \end{aligned}$$

$$\psi(\vec{r}, \vec{p}) = \frac{1}{V} \int d\vec{r} e^{-\frac{\pi}{\lambda T^2} \left(r^2 - i \frac{\lambda T}{2\pi} \vec{p} \cdot \vec{r} \right)^2} e^{-\frac{\lambda T^2}{4\pi^2} p^2}$$



If I add these two, then you see the this particular term is identical to this and therefore, the exponential is π over λT square r minus $i \vec{p} \lambda T$ square over 2π whole square plus λT square over 2π whole square times p^2 which is going to be e to the power minus π over λT square r minus $i \lambda T$ square over 2π times p whole square minus π over λT square and I have λT raised to the power $4\pi^2 p^2$.

So, this gives me lambda T square and then, I have a pi over here so that I have e to the power minus pi over lambda T square r minus i lambda T square over 2 pi times p whole square e to the power minus lambda T square over 4 pi times p square. Therefore, rho of R comma p is 1 by v and then, I have d of r e to the power minus pi lambda T square r minus i lambda T square over 2 pi times p square e to the power minus lambda T square over 4 pi times p square.

However, note that I have made a severe mistake in the sense that I did not include a h bar over here. So, if I have to include a h bar over here that means, this becomes h bar right, this becomes 2 pi is replaced by 2 pi h bar, you have a h bar, you have a h bar and here, you have h bar square again, you have h bar square, h bar square.

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$$\begin{aligned}
 \rho(\vec{r}, \vec{p}) &= \frac{1}{V} \int d\vec{r}' e^{-i\lambda_T^2 (r - \vec{r}') \cdot \vec{p}} e^{-\frac{\lambda_T^2}{4\pi^2} p^2} \\
 &= \frac{1}{V} e^{-\frac{\lambda_T^2}{4\pi^2} p^2} \int d\vec{r}' e^{-\pi i \lambda_T^2 (\vec{r} - \vec{r}') \cdot \vec{p}} \\
 &= \frac{1}{V} e^{-\frac{\lambda_T^2}{4\pi^2} p^2} \left(\sqrt{\frac{\pi}{\lambda_T^2}} \right)^3 = \frac{1}{V} \lambda_T^3 e^{-\frac{\lambda_T^2}{4\pi^2} p^2} \\
 &= \frac{\lambda_T}{V} e^{-\frac{\lambda_T^2}{4\pi^2} p^2}
 \end{aligned}$$



So, now, therefore, I have 1 over v lambda T square over $4 \pi h \bar{}$ square times p square, I have dr e to the power minus π over lambda T square r minus r_0 whole square and this is clearly a Gaussian integral and remember this has a measure of r square so, therefore, you come up with the result that this is going to be 1 by v e to the power minus lambda T square over $4 \pi h \bar{}$ square p square.

And this is square root π over lambda T whole square raised to the power 3 my mistake sorry, this has to be π times lambda T square raised to the power 3 which is equal to 1 by v , you have lambda T whole cube e to the power minus lambda T square over $4 \pi h \bar{}$ square p square good. So, this becomes you see the thermal volume times e to the power minus lambda T square over $4 \pi h \bar{}$ square p square.

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$$\begin{aligned}
 &= \frac{1}{V} e^{-\frac{\lambda_T^2}{4m^2} \beta^2} \left(\sqrt{\frac{\pi}{\lambda_T}} \lambda_T \right)^3 = \frac{1}{V} \lambda_T^3 e^{-\frac{\lambda_T^2}{4m^2} \beta^2} \\
 &= \frac{\lambda_T}{V} e^{-\frac{\lambda_T^2}{4m^2} \beta^2} \\
 &\lambda_T = \left(\frac{\beta h^2}{2m\pi} \right)^{1/2} \quad \lambda_T^2 = \frac{\beta h^2}{2m\pi} \quad h^2 = 4\pi^2 \hbar^2 \\
 &\frac{\beta h^2}{2m} \cdot \frac{1}{4\pi^2 \hbar^2} \\
 &\int \frac{4\pi^2 \hbar^2}{4\pi^2 \hbar^2} = \frac{\beta}{2m}
 \end{aligned}$$

Canonical phase space density:

$$f(\vec{R}, \vec{p}) = \frac{\lambda_T}{V} e^{-\beta \frac{p^2}{2m}}$$



Now, let us focus on this term. So, now, λT is $\beta \hbar$ over $2m \pi$ raised to the power half. So, that λT square is going to be β so, this has to be \hbar square; \hbar square over twice $m \pi$. So, let us rewrite this. Now, therefore, as $\beta \hbar$ square over twice $m \pi$ times 1 over $4 \pi \hbar$ square which we will write down as 1 over 4π square \hbar square and \hbar square I note is that 2π times not 2π , but 4π square times \hbar square.

Therefore, this is β over twice $m 4 \pi$ square \hbar square divided by 4π square \hbar square so that this is β over $2m$. So, essentially what you have is R , this ρ of R, p , the classical observable corresponding to the phase space to the quantum mechanical operator ρ hat gives you the classical observable which is λT over v that follows from this relation e to the power minus βp square over $2m$.

And this is exactly the canonical phase space density that we derived when we did classical statistical mechanics.

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$O_{cl}(\vec{r}, \vec{p}) \leftrightarrow \langle \vec{r}' | \hat{O} | \vec{r} \rangle = \frac{1}{h^3} \int d\vec{p}' O_{cl}(\frac{\vec{r}+\vec{r}'}{2}, \vec{p}') e^{i\vec{p}' \cdot (\vec{r}-\vec{r}')/\hbar}$
 $O_{cl} \rightarrow \rho(\vec{r}, \vec{p}) = \left(\frac{\lambda T}{v} \right) e^{-\beta \vec{p}^2 / 2m}$
 $\langle \vec{r}' | \hat{O} | \vec{r} \rangle = \frac{1}{h^3} \int d\vec{p}' \frac{\lambda T}{v} e^{-\beta \vec{p}'^2 / 2m} e^{i\vec{p}' \cdot (\vec{r}-\vec{r}')/\hbar}$

$$-\frac{\beta}{2m} \left[\vec{p}'^2 - 2 \frac{i m \vec{p}' \cdot (\vec{r}-\vec{r}')}{\hbar} \right]$$

$$-\frac{\beta}{2m} \left[\left(\vec{p}' - \frac{i m (\vec{r}-\vec{r}')}{\hbar} \right)^2 - \left(\frac{i m}{\hbar} \right)^2 (\vec{r}-\vec{r}')^2 \right]$$

$$-\frac{\beta}{2m} \left(\vec{p}' - \frac{i m}{\hbar} \right)^2 - \frac{\beta}{2m} \frac{m^2}{\hbar^2} (\vec{r}-\vec{r}')^2$$



So, now let us apply the reverse. So, we want to use the well quantization principle and essentially that says that if I have a classical operator r, p I can get the corresponding matrix element of the quantum mechanical operator in the coordinate representation as $\frac{1}{h^3} \int dp O_{cl}(r, p)$, this is r plus r' by 2 p e to the power $i p \cdot r' - r$ over h bar.

And in our case, I know that O_{cl} corresponds to ρ , the phase space density which goes as $\frac{\lambda T}{v} e^{-\beta p^2 / 2m}$. So, that essentially, I have O_{cl} as $\frac{1}{h^3} \int dp e^{-\beta p^2 / 2m} e^{i p \cdot (r' - r) / \hbar}$ good, it is the same trick. So, this is a vector integral.

So, it is the same trick now, we take these two and write this as $\frac{\beta}{2m} p^2$ minus $2 i m \beta \hbar^{-1} r \cdot r' - r$ p dot right which becomes minus β

over twice m I have p, vector p minus i m over beta h bar r prime minus r whole square and then, I have minus i m beta h bar whole square r prime minus r whole square.

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$$\begin{aligned}
 & -\frac{\beta}{2m} \left[\left(\vec{p} - \frac{im}{\beta \hbar} (\vec{r}' - \vec{r}) \right) - \left(\frac{2m}{\beta \hbar} (\vec{r}' - \vec{r}) \right) \right] \\
 & -\frac{\beta}{2m} (\vec{p} - \vec{p}_0)^2 - \frac{\beta}{2m} \frac{m^2}{\beta^2 \hbar^2} (\vec{r}' - \vec{r})^2 \\
 & -\frac{\beta}{2m} (\vec{p} - \vec{p}_0)^2 - \frac{m}{2\beta \hbar^2} (\vec{r}' - \vec{r})^2 \\
 \langle \vec{r}' | \hat{p} | \vec{r} \rangle &= \frac{1}{h^3} \frac{\lambda_T}{V} \int d\vec{p} e^{-\frac{\beta}{2m} (\vec{p} - \vec{p}_0)^2} e^{-\frac{m}{2\beta \hbar^2} (\vec{r}' - \vec{r})^2} \\
 &= \frac{\lambda_T}{V} \frac{1}{h^3} \left(\sqrt{\frac{2m\hbar}{\beta}} \right)^3 e^{-\frac{m}{2\beta \hbar^2} (\vec{r}' - \vec{r})^2}
 \end{aligned}$$



So, that this becomes very nicely p minus p 0 whole square and then, I have a minus, minus makes it a plus, but then, I have i square which makes it a minus, I have m square over beta h bar square r prime minus r whole square times beta over twice m. So, that this becomes beta over 2m p minus p 0 whole square minus this beta, beta gets cancelled, m sorry it gives me 1 power of beta because this is beta square over here, I get m over here and then, I get 2 beta h bar square r prime minus r whole square.

So, that the matrix representation, matrix elements in the coordinate representation of this operator rho becomes 1 by h cube, there is something which we have missed, we have missed this factor which will come in over here which is going to be lambda T over v. So, I have

lambda T over v and then, I have integral over dp e to the power minus beta over twice m pi minus p naught whole square e to the power minus m over 2 beta h bar square r prime minus r whole square right.

This is a standard Gaussian integral which we have been doing so much so that I can immediately write down this as 1 over h cube square root pi so, this is going to be square root twice m pi over beta raised to the power 3 and then, I will have e to the power m over 2 beta h bar square r prime minus r whole square.

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$$\begin{aligned}
 \langle \vec{r}' | \hat{f} | \vec{r} \rangle &= \frac{1}{h^3} \frac{\Lambda_T}{V} \int d\vec{p} e^{-\frac{\beta}{2m} (\vec{p} - \vec{p}_0)^2} e^{-\frac{m}{2\beta h^2} (\vec{r}' - \vec{r})^2} \\
 &= \frac{\Lambda_T}{V} \frac{1}{h^3} \left(\sqrt{\frac{2m\pi}{\beta}} \right)^3 e^{-\frac{m}{2\beta h^2} (\vec{r}' - \vec{r})^2} \\
 &= \frac{\Lambda_T}{V} \frac{1}{\Lambda_T} e^{-\frac{\pi^2}{\lambda_T^2} (\vec{r}' - \vec{r})^2} \quad \left(\lambda_T = \left(\frac{\beta h^2}{2m\pi} \right)^{1/2} \right) \\
 \langle \vec{r}' | \hat{f} | \vec{r} \rangle &= \frac{1}{V} e^{-\frac{\pi^2}{\lambda_T^2} (\vec{r}' - \vec{r})^2} \quad \left(\frac{m^2 h^2}{2\beta h^2} = \pi \frac{2m\pi}{\beta h^2} \frac{\pi}{\lambda_T^2} \right)
 \end{aligned}$$



Now, recall that the thermal de Broglie wavelength lambda T was beta h over twice m pi half right and if you look at this expression, then this is going to be m 2 beta times h square 4 pi square. So, which we write down as pi, this gives me 2, 2m pi beta h square.

So, this is the mistake I made in the earlier expression and you immediately see that this is going to be π over λT whole square and this together is going to give you the inverse of the thermal volume and you will cover the result π square over λT square r prime minus r whole square.

So, that you have the result which we derived when we looked at the ideal gas the inter coordinate representation that the density matrix look like this. So, therefore, we have now very nice way of going from the classical to the corresponding quantum mechanical representation. So, given a classical operator, we can go to the quantum mechanical operator or given a quantum mechanical operator, we can go to the classical operator.