Semi-classical thermodynamics of a non-interacting gas in a periodic potential

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October 2013

Contents

1 Tight-binding Approximation

The hamiltonian of a 1D lattice is[1]

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V_0 \sum_{i=1}^{3} \cos^2\left(\pi \hat{x}_i / d\right) + \frac{1}{2} m\omega^2 \sum_{i=1}^{3} \hat{x}_i^2. \tag{1}$$

Expansion in terms of localized Wannier functions. Bloch wavefunction $\phi_k(x) =$

[1] Explain what the semi-classical approximation is, like in Pethick p.28. In the context of a BEC in a harmonic trap, the semi-classical approximation is valid when $k_B T \gg \hbar\omega$ or, equivalently, when $\lambda_T = h/\sqrt{2\pi m k_B T} \ll a_{\text{ho}} = \sqrt{\hbar/(m\omega)}$.

$\frac{1}{\sqrt{N}}\sum_n e^{iknd}w(x-nd)$ where k is related to the quasimomentum q by $k=\frac{q}{\hbar}$

$$\begin{aligned}E(k,x) &= \langle\hat{H}\rangle \\ &= \int dx'\,\phi^*(x')H_0(x')\phi(x') + \frac{1}{2}m\omega^2x^2 \\ &= \frac{1}{N}\sum_{n,n'} e^{ik(n-n')d}\int dx'\,w^*(x'-nd)H_0(x')w(x'-n'd) + \frac{1}{2}m\omega^2x^2, \qquad (2)\end{aligned}$$

where $H_0(x)\equiv -\frac{\hbar^2}{2m}\nabla^2 + V_0\cos^2(\pi x/d)$. In the tight-binding approximation, the sum over n' is truncated to the nearest-neighbor terms, $n'=n, n\pm 1$. Defining $\epsilon_0\equiv\int dx'\,w^*(x')H_0(x')w(x')$ and $t\equiv -\int dx'\,w^*(x')H_0(x')w(x'-d)$, and using the periodicity of the potential, we have

$$\begin{aligned}E(k,x) &= \frac{1}{N}\sum_n\left[\epsilon_0 - te^{-ikd} - te^{ikd}\right] + \frac{1}{2}m\omega^2x^2 \\ &= \epsilon_0 - 2t\cos(kd) + \frac{1}{2}m\omega^2x^2. \qquad (3)\end{aligned}$$

It is convenient to set the minimum of the energy to zero. Therefore,

$$E(k,x) = 2t\left[1-\cos(kd)\right] + \frac{1}{2}m\omega^2x^2. \qquad (4)$$

We can extend the results to a 3D potential

$$E(q_x,q_y,q_z,x,y,z) = 2t\sum_{i=1}^{3}\left[1-\cos(\pi q_i/q_B)\right] + \frac{1}{2}m\omega^2\sum_{i=1}^{3}x_i^2, \qquad (5)$$

where $q_i\equiv\hbar k$ is the quasimomentum and $q_B\equiv\frac{\hbar\pi}{d}$. In the next section we will integrate over q_i and x_i. Recall that there is a prefactor $\frac{1}{h}$ associate with each differential pair $dx_i\,dq_i$.

1.1 Quasimomentum distribution

$$\begin{aligned}n_{\mathrm{ex}}(q_x,q_y,q_z) &= \frac{1}{h^3}\int d^3r\,\frac{1}{z^{-1}e^{\beta E(q_x,q_y,q_z,x,y,z)}\mp 1} \\ &= \frac{4\pi}{h^3}\int_0^\infty dr\,r^2\frac{1}{z^{-1}e^{2\beta t\sum_i[1-\cos(\pi q_i/q_B)]}e^{\frac{1}{2}\beta m\omega^2r^2}\mp 1} \qquad (6)\end{aligned}$$

where $z \equiv e^{\beta\mu}$ is the fugacity and the $\mp$ sign corresponds to bosons/fermions.

Making the change of variables $u \equiv \frac{\beta m\omega^2 r^2}{2} \Rightarrow r = \sqrt{\frac{2u}{\beta m\omega^2}}$ and $dr = \frac{du}{\sqrt{2\beta m\omega^2 u}}$ leads to

$$n_{\text{ex}}(q_x, q_y, q_z) = \frac{2\pi}{h^3}\left(\frac{2}{\beta m\omega^2}\right)^{3/2}\int_0^\infty du\,\frac{\sqrt{u}}{z^{-1}e^{2\beta t\sum_i[1-\cos(\pi q_i/q_B)]}e^u \mp 1}. \tag{7}$$

The integral can be written as $\pm\frac{\sqrt{\pi}}{2}\text{Li}_{3/2}(\pm z e^{-2\beta t\sum_i[1-\cos(\pi q_i/q_B)]})$, where Li is a polylogarithm function[2]. Therefore,

$$\begin{aligned} n_{\text{ex}}(q_x, q_y, q_z) &= \pm\frac{1}{\hbar^3(2\pi\beta m\omega^2)^{3/2}}\text{Li}_{3/2}(\pm z e^{-2\beta t\sum_i[1-\cos(\pi q_i/q_B)]}) \\ &= \boxed{\pm\left(\frac{a_{\text{ho}}^2}{\hbar\lambda_T}\right)^3\text{Li}_{3/2}(\pm z e^{-2\beta t\sum_i[1-\cos(\pi q_i/q_B)]})}, \end{aligned} \tag{8}$$

where $a_{\text{ho}} \equiv \sqrt{\frac{\hbar}{m\omega}}$ is the characteristic length of the harmonic trap and $\lambda_T \equiv \sqrt{\frac{2\pi\hbar^2}{mk_BT}}$ is the de Broglie wavelength. Note that $n(q_x, q_y, q_z)$ has units of volume.

1.2 Non-condensed atom number

Integrating eq. (8) over the first Brillouin zone gives

$$N_{\text{ex}} = \pm\left(\frac{a_{\text{ho}}^2}{\hbar\lambda_T}\right)^3\int d^3q\,\text{Li}_{3/2}(\pm z e^{-2\beta t\sum_i[1-\cos(\pi q_i/q_B)]}). \tag{9}$$

The polylogarithm function can be expressed as a series[3], resulting in

$$N_{\text{ex}} = \pm\left(\frac{a_{\text{ho}}^2}{\hbar\lambda_T}\right)^3\sum_{n=1}^{\infty}\frac{(\pm z)^n e^{-6\beta t n}}{n^{3/2}}\left(\int_{-q_B}^{q_B} dq\,e^{2\beta t n\cos(\pi q/q_B)}\right)^3. \tag{10}$$

Under the change of variables $\theta \equiv \pi q/q_B$, the integral becomes $2q_B/\pi\int_0^\pi d\theta\,e^{2\beta t n\cos\theta}$, which can be expressed in terms of modified Bessel functions of the first kind[4], we find

$$\boxed{N_{\text{ex}} = \pm 8\pi^3\left(\frac{a_{\text{ho}}^2}{\lambda_T\,d}\right)^3\sum_{n=1}^{\infty}\frac{(\pm z)^n e^{-6\beta t n}I_0^3(2\beta t n)}{n^{3/2}}}. \tag{11}$$

[2] $\text{Li}_s(\pm z) \equiv \pm\frac{1}{\Gamma(s)}\int_0^\infty du\,\frac{u^{s-1}}{z^{-1}e^u \mp 1}$

[3] $\text{Li}_s(z) = \sum_{n=1}^{\infty}\frac{z^n}{n^s}$

[4] $I_n(z) \equiv \frac{1}{\pi}\int_0^\pi d\theta\,e^{z\cos\theta}\cos n\theta$

1.3 Potential energy

$$
\begin{aligned}
\bar{U} &= \left\langle \frac{1}{2} m\omega^2 r^2 \right\rangle \\
&= \frac{2\pi m\omega^2}{h^3} \int d^3q \int_0^\infty dr\, r^4 \frac{1}{z^{-1} e^{2\beta t \sum_i [1-\cos(\pi q_i/q_B)]} e^{\beta m\omega^2 r^2/2} \mp 1} \\
&= \frac{\pi m\omega^2}{h^3} \left(\frac{2}{\beta m\omega^2}\right)^{5/2} \int d^3q \int_0^\infty du \frac{u^{3/2}}{z^{-1} e^{2\beta t \sum_i [1-\cos(\pi q_i/q_B)]} e^{u} \mp 1} \\
&= \pm \frac{\pi m\omega^2}{h^3} \left(\frac{2}{\beta m\omega^2}\right)^{5/2} \frac{3\sqrt{\pi}}{4} \int d^3q\, \mathrm{Li}_{5/2}(\pm z e^{-2\beta t \sum_i [1-\cos(\pi q_i/q_B)]}) \\
&= \pm \frac{6(2\pi)^{3/2} m\omega^2}{4h^3} \left(\frac{1}{\beta m\omega^2}\right)^{5/2} \int d^3q\, \mathrm{Li}_{5/2}(\pm z e^{-2\beta t \sum_i [1-\cos(\pi q_i/q_B)]}) \\
&= \pm \frac{12 q_B^3}{(2\pi\beta m\omega^2)^{3/2} \beta \hbar^3} \sum_{n=1}^\infty \frac{(\pm z)^n e^{-6\beta t n} I_0^3(2\beta t n)}{n^{5/2}} \\
&= \boxed{\pm \frac{12\pi^3}{\beta} \left(\frac{a_{\mathrm{ho}}^2}{\lambda_T\, d}\right)^3 \sum_{n=1}^\infty \frac{(\pm z)^n e^{-6\beta t n} I_0^3(2\beta t n)}{n^{5/2}}}. \qquad (12)
\end{aligned}
$$

1.4 Kinetic energy

$$
\begin{aligned}
\bar{K} &= \int d^3q\, 2t \sum_i [1-\cos(\pi q_i/q_B)]\, n(q_x, q_y, q_z) \\
&= 6tN_{\mathrm{ex}} - 6t \int dq^3\, \cos(\pi q_x/q_B)\, n(q_x, q_y, q_z). \qquad (13)
\end{aligned}
$$

The last integral equals

$$
\begin{aligned}
&= \pm \frac{1}{(2\pi\beta m\omega^2)^{3/2}\hbar^3} \int d^3q\, \cos(\pi q_x/q_B)\, \mathrm{Li}_{3/2}(\pm z e^{-2\beta t \sum_i [1-\cos(\pi q_i/q_B)]}) \\
&= \pm \frac{1}{(2\pi\beta m\omega^2)^{3/2}\hbar^3} \sum_{n=1}^\infty \frac{(\pm z)^n e^{-6\beta t n}}{n^{3/2}} \left(\int dq\, e^{2\beta t n \cos(\pi q_i/q_B)}\right)^2 \cdot \\
&\quad \cdot \int dq\, \cos(\pi q/q_B)\, e^{2\beta t n \cos(\pi q/q_B)} \\
&= \pm \frac{8 q_B^3}{(2\pi\beta m\omega)^{3/2}\hbar^3} \sum_{n=1}^\infty \frac{(\pm z)^n e^{-6\beta t n} I_1(2\beta t n) I_0^2(2\beta t n)}{n^{3/2}}. \qquad (14)
\end{aligned}
$$

Therefore,

$$\begin{aligned}\mathrm{KE} &= \pm\frac{6t\cdot 8\,q_B^3}{(2\pi\beta m\omega)^{3/2}\hbar^3}\sum_{n=1}^{\infty}\frac{(\pm z)^n e^{-6\beta tn} I_0^2(2\beta tn)\,[I_0(2\beta tn)-I_1(2\beta tn)]}{n^{3/2}}\\ &= \boxed{\pm 48\,t\left(\frac{a_{\rm ho}^2}{\lambda_T\,d}\right)^3\sum_{n=1}^{\infty}\frac{(\pm z)^n e^{-6\beta tn} I_0^2(2\beta tn)\,[I_0(2\beta tn)-I_1(2\beta tn)]}{n^{3/2}}}.\end{aligned} \tag{15}$$

1.5 Grand potential

The grand potential is [5]

$$\begin{aligned}\Omega &= \pm\frac{1}{\beta h^3}\int d^3r\int d^3q\,\ln\left(1\mp z e^{-\beta E(q_x,q_y,q_z,x,y,z)}\right)\\ &= \pm\frac{4\pi}{\beta h^3}\int_0^{\infty} dr\,r^2\int d^3q\,\ln\left(1\mp z e^{-2\beta t\sum_i[1-\cos(\pi q_i/q_B)]-\frac{1}{2}\beta m\omega^2 r^2}\right).\end{aligned} \tag{16}$$

Expanding the natural logarithm[6] leads to

$$\Omega = \mp\frac{4\pi}{\beta h^3}\sum_{n=1}^{\infty}\frac{(\pm z)^n e^{-6\beta tn}}{n}\int_0^{\infty} dr\,r^2 e^{-\frac{n\beta m\omega^2 r^2}{2}}\int d^3q\,e^{2\beta tn\sum_i\cos(\pi q_i/q_B)}. \tag{17}$$

The first and second integrals are $\frac{\sqrt{2\pi}}{2(n\beta m\omega^2)^{3/2}}$ and $8q_B^3 I_0^3(2\beta tn)$ respectively, therefore,

$$\begin{aligned}\Omega &= \mp\frac{8q_B^3}{(2\pi\beta m\omega^2)^{3/2}\beta\hbar^3}\sum_{n=1}^{\infty}\frac{(\pm z)^n e^{-6\beta tn} I_0^3(2\beta tn)}{n^{5/2}}\\ &= \boxed{\mp\frac{8\pi^3}{\beta}\left(\frac{a_{\rm ho}^2}{\lambda_T\,d}\right)^3\sum_{n=1}^{\infty}\frac{(\pm z)^n e^{-6\beta tn} I_0^3(2\beta tn)}{n^{5/2}}}.\end{aligned} \tag{18}$$

1.6 Entropy

The entropy is given by

$$S = \frac{E-\mu N-\Omega}{T}, \tag{19}$$

where N is the *total* atom number.

[5] The grand canonical potential is given by the formula $\Omega = -\beta^{-1}\ln\prod_{\lambda=1}^{\infty}\xi_\lambda$, with $\xi_\lambda = \sum_{N_\lambda=0}^{\infty} e^{-\beta N_\lambda(\epsilon_\lambda-\mu)}$. In the case of bosons $\xi = (1-ze^{-\beta\epsilon_\lambda})^{-1}$; in the case of fermions $\xi = 1+ze^{-\beta\epsilon_\lambda}$. Hence, $\Omega = \pm\beta^{-1}\sum_{\lambda=1}^{\infty}\ln(1\mp ze^{-\beta\epsilon_\lambda})$ for bosons/fermions.

[6] $\ln(1+x) = \sum_{n=1}^{\infty}\frac{(-1)^{n+1}x^n}{n} \qquad \text{for} \quad -1 < x \leq 1$

2 Numerical calculations

The following plots show the condensate fraction N_0/N and the entropy per particle S/N versus the temperature T. Total atom number $N = 10^5$, trap frequency $\omega = (2\pi)40\text{Hz}$, tunneling energy $t = 0.086\ \text{E}_R$ (lattice depth $= 4\ \text{E}_R$).

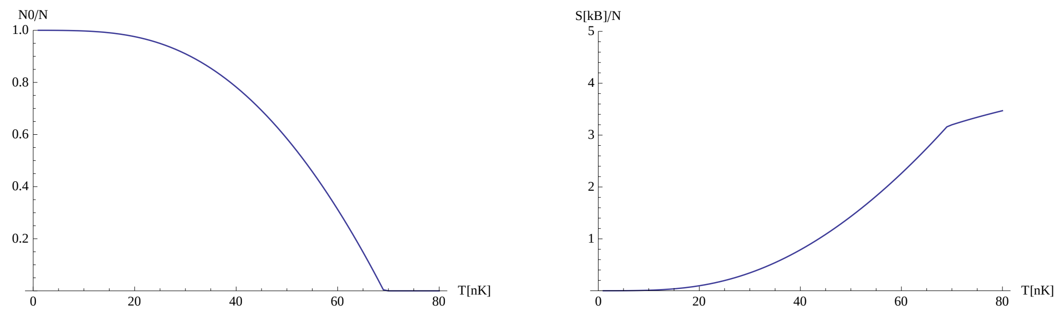

Figure 1: Condensate fraction N_0/N (left) and entropy per particle S/N (right) vs temperature T.

The next plots show the gas temperature T, the critical temperature T_c and the condensate fraction N_0/N as the lattice depth is increased in an isentropic process[7]. The initial temperature is 50 nK and the total atom number is $N = 10^5$. Trap frequency $\omega = (2\pi)40\text{Hz}$.

[7] The second law of thermodynamics states $dS \geq dQ/T$. The equality holds for a reversible process. Hence, isentropic is the same as reversible adiabatic.

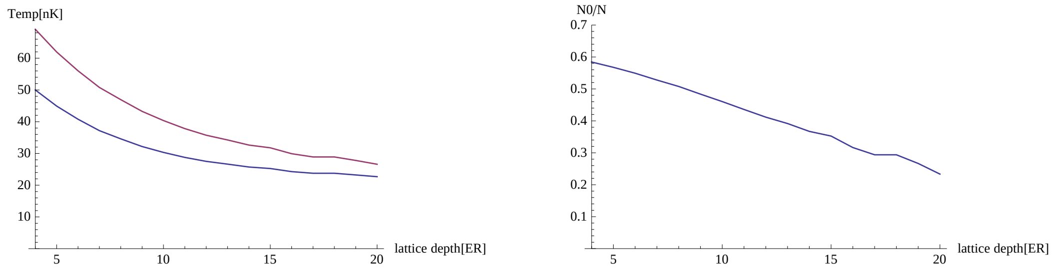

Figure 2: Gas temperature T (left, blue), critical temperature T_c (left, red) and condensate fraction N_0/N(right) versus lattice depth s. Intuitively speaking, T drops as s increases because of an effective-mass effect. On the left plot we observe that T_c (red) drops faster than T (blue) and, therefore, the N_0/N decreases. This is qualitatively consistent with the behavior seen experimentally.

The gas temperature T as the trap frequency ω increases isentropically. Tunneling energy $t = 0.086$ E$_R$

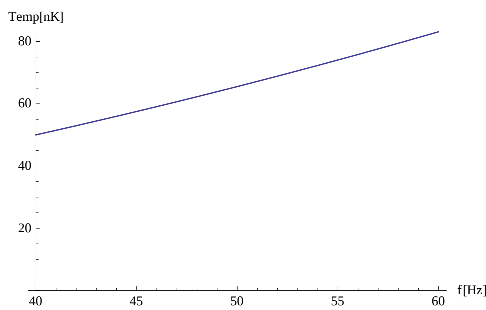

Figure 3: As expected, T rises as the gas gets compressed.

In our apparatus, there are two effects with the opposite sign as the lattice depth increases. First, the trap frequency increases due to the gaussian nature of the red-detuned lattice beams and, therefore, the gas temperature decreases. Second, the gas temperature decreases because of an effective-mass effect.