1 The upshot

In our experiment we will create a three-dimensional optical lattice for confining metastable Helium (He*). The lattice trap exploits the ıdipole force due to the spatial variation of the atomic internal energy. This spatial dependence arises from the light shift, or AC Stark effect, which in an optical lattice varies periodically in an optical standing wave created by retro-reflected laser beams. In this brief report we will learn a few things about the confining potential, the lattice parameters U and J (and J as a function of position), the tunnelling time, and the band structure of our lattice.

A few figures to keep in mind:

$2^3S_1 \rightarrow 2^3P_2$ **transition wavelength** 1083.331 nm

$2^3S_1 \rightarrow 2^3P_2$ **transition frequency** 2π 276 THz

$2^3S_1 \rightarrow 2^3P_2$ **transition** 2π 1.6 MHz

Lattice wavelength 1550 nm

Lattice frequency 2π 192.9 THz

Mass of He4 6.649E-27 kg = 4.003 amu = 3.71 GeV/c^2

He* scattering length 7.512 nm

2 The Dipole Force

We follow the method in Metcalf and van der Straten's book [5] in what immediately follows. We begin with the time-dependent Schrödinger equation,

$$\hat{H}|\psi(x,t)\rangle = i\hbar\frac{\partial}{\partial t}|\psi(x,t)\rangle$$

for any ket $|\psi(x,t)\rangle$ and (possibly time-dependent) hamiltonian $\hat{H}$. If $|\phi_i(x,t)\rangle$ are a complete set of eigenstates of the Hamiltonian with energy E_i then we can write $|\psi(x,t)\rangle$ as a linear combination of these eigenvectors;

$$|\psi(x,t)\rangle = \sum_i c_i|\phi_i(x,t)\rangle \tag{1}$$

where the c_i may in general be time-dependent. Then the TDSE for a single eigenstate shows

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\phi_i(x,t)\rangle &= E_i|\phi_i(x,t)\rangle \\ \implies |\psi_i(x,t)\rangle &= e^{-iE_it/\hbar}|\phi_i(x,0)\rangle \\ &= e^{-i\omega_i t}|\phi_i\rangle \end{aligned} \tag{2}$$

Where we write $|\phi_i\rangle$ as shorthand for $|\phi_i(x,0)\rangle$ and $E_i = \hbar\omega_i$. Thus

$$|\psi(x,t)\rangle = \sum_i c_i(t) e^{-iE_i t}|\phi_i\rangle \tag{3}$$

Consider, then, a hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}'$, where $\hat{H}_0$ is fully diagonal with eigenvectors $|\phi_i\rangle$ and $\hat{H}'$ has zero diagonal elements. That is, we separate the Hamiltonian into atomic motion and interaction components. Below we assume the interaction is mediated by the photon field created by the application of laser light. Then, the Schrödinger equation for the system becomes

$$\begin{aligned}(\hat{H}_0 + \hat{H}')\sum_j e^{-i\omega_j t} c_j(t)|\phi_j\rangle &= i\hbar\frac{\partial}{\partial t}\sum_j e^{-i\omega_j t} c_j(t)|\phi_j\rangle \\ &= \sum_j \Big(E_j c_j(t) + i\hbar\frac{dc_j(t)}{dt}\Big) e^{-i\omega_j t}|\phi_j\rangle\end{aligned} \tag{4}$$

If we contract the left hand side by multiplying through another eigenket $\langle\phi_k(x,t)| = \langle\phi_k|e^{i\omega_k t}$, we find

$$\begin{aligned}\sum_j e^{i(\omega_k-\omega_j)t} c_j(t)\langle\phi_k|(\hat{H}_0 + \hat{H}')|\phi_j\rangle &= \sum_j e^{i(\omega_k-\omega_j)t} c_j(t)\big(E_j\delta_{j,k} + \langle\phi_k|\hat{H}'|\phi_j\rangle\big) \\ &= E_k c_k(t) + \sum_j e^{i(\omega_k-\omega_j)t} c_j(t)\langle\phi_k|\hat{H}'|\phi_j\rangle\end{aligned} \tag{5}$$

Whereas on the right we have

$$\sum_j \Big(E_j c_j(t) + i\hbar\frac{dc_j(t)}{dt}\Big) e^{i(\omega_k-\omega_j)t}\langle\phi_k|\phi_j\rangle = E_k c_k(t) + i\hbar\frac{dc_k(t)}{dt} \tag{6}$$

Equating these sides once more we find the governing equation for the time evolution of the complex amplitudes $c_i(t)$;

$$\begin{aligned}i\hbar\frac{dc_k(t)}{dt} &= \sum_j e^{i(\omega_k-\omega_j)t} c_j(t)\langle\phi_k|\hat{H}'|\phi_j\rangle \\ &= \sum_j e^{i\omega_{kj}t} c_j(t)\hat{H}'_{kj}\end{aligned} \tag{7}$$

Where the shorthand is evident. If we restrict our attention to a two-level system with excited and ground states $|e\rangle$ and $|g\rangle$, respectively, then we find the evolution equations for the amplitude of each state

$$\begin{aligned}i\hbar\frac{dc_g(t)}{dt} &= e^{-i\omega_0 t} c_e(t)\hat{H}'_{ge} \\ i\hbar\frac{dc_e(t)}{dt} &= e^{i\omega_0 t} c_g(t)\hat{H}'_{eg}\end{aligned} \tag{8}$$

Where $\omega_0 = \omega_e - \omega_g$ is the *resonant frequency* of the transition, sometimes referred to simply as the *resonance*.

We now fix the Hamiltonian as that of an atom in a magnetic field,

$$\hat{H} = \frac{(\hat{p} - (e/c)\vec{A})^2}{2m} + \hat{V}, \tag{9}$$

and after some consternation the following expression can be found for the perturbative Hamiltonian

$$\hat{H}' = -e\Lambda(\vec{(r)}, t) \cdot \vec{(r)} \tag{10}$$

Where $\Lambda = \dot{\vec{A}}/c$. If Metcalf and van der Straten are anyone to trust, the derivation of this innocuous equation took forty years of trouble to conclude. The present author resents this complication. And so on, we end up deriving the following shifts in internal energy states;

$$\begin{aligned} \Delta E_g &= \frac{\hbar\Omega^2}{4\delta} \\ \Delta E_e &= -\frac{\hbar\Omega^2}{4\delta} \end{aligned} \tag{11}$$

As these shifts are proportional to Ω^2 and hence optical intensity, this phenomenon is referred to as the light shift.

3 Lattice structure

And after some time we find an expression for the lattice potential

$$V_{Lat} = \frac{3\pi c^2}{2{\omega_0}^3} \frac{\Gamma}{\delta} \frac{2P}{\pi {w_0}^2} \tag{12}$$

which is useful to express in terms of $E_r = \hbar^2 k^2/2m$, the recoil energy (the energy imparted by a single scattered photon). δ is the detuning from resonance, Γ is the natural linewidth, w_0 is the beam waist size and P is the total laser power. This approximation is valid when the laser detuning is large compared to the transition fine-structure splitting. Assuming our lattice parameters and 4W beams with 100micron waists, we expect to be able to generate lattice depths of order $30E_r$.

In Morsch and Oberthaler [6] there is an expression given involving some Clebsch-Gordon coefficients (which might wind up the same, after some approximations?) $V_0 = \zeta\hbar\Gamma\frac{I_p}{I_0}\frac{\Gamma}{\Delta}$, where ζ depends on the atomic level structure through the Clebsh-Gordan coefficients.

In a full 3D lattice the optical potential has the form

$$V(\vec{x}) = -\sum_{i=1}^{3} V_{x_i} e^{-2\frac{\vec{r_i}^2}{{w_i}^2}} \sin^2(kx_i) \tag{13}$$

Where the $\vec{r_i}$ are the smallest perpendicular distance from the axis of the i^{th} beam, and w_i is its beam waist size. For traps very close to the beam axes, the following linearization is useful

$$V(\vec{x}) = -\sum_{i=1}^{3} \Big(V_{x_i} \sin^2(kx_i) + \frac{m}{2}(\omega_i x_i)^2 \Big) \tag{14}$$

Where the second term corresponds to the global harmonic trapping by the Gaussian beam.

In an isotropic lattice,

$$\omega_{lat}^2 = V_{lat} \frac{2k^2}{m} = \frac{V_{lat}}{E_r} \frac{\hbar^2 k^4}{m^2} \tag{15}$$

are the trapping frequencies of the lattice sites. At the centre of our lattice we should achieve trapping frequencies up to 1.4MHz at individual lattice sites.

However the spatial variation in beam intensity leads to a position-dependent trapping frequency and spatially-varying ground states (c.f. $V_{GS} = \frac{\hbar}{2}(\hbar^2 \vec{k}(\vec{x}) \cdot \vec{k}(\vec{x})))$ More specifically, along the x-axis for example, the trapping frequencies vary as

$$\begin{aligned} \omega_{lat_x}(x) &= \omega_{lat_x}(0) e^{-\frac{y^2+z^2}{w_x^2}} \\ &\approx \omega_{lat_x}(0)\big(1 - \frac{y^2+z^2}{w_x^2}\big) \end{aligned} \tag{16}$$

The global confining potential from the Gaussian beam, and the corresponding overall trap frequency, are given by

$$\begin{aligned} V_{ext} &= E_r \frac{2r^2}{w_0^2}\big(2\frac{V_l}{E_r} - \sqrt{\frac{V_l}{E_r}}\big) \\ \omega_{ext}^2 &= \frac{4E_r^2}{m w_0}\big(2\frac{V_l}{E_r} - \sqrt{\frac{V_l}{E_r}}\big) \end{aligned} \tag{17}$$

Thus we expect an overall harmonic trap frequency of

4 Lattice parameters

We may find [4] useful, as it prescribes a numerical method for computing single-particle band structure in a lattice BEC, with varying interaction and optical potential terms. Probably the go-to for our method, but we need a root-finding operation.

We will also see some use of Bloch et al [2], as in their detailed review they state the following relationship between tunnelling parameters (for a given band) and the energies of that band;

$$\sum_{\vec{R}} J_n(\vec{R}) e^{i\vec{q}\cdot\vec{R}} = \epsilon_n(\vec{q} \tag{18}$$

where $\epsilon_n(\vec{q})$ are the Bloch band energies, and $\vec{R}$ addresses the lattice sites (i.e. it's a lattice vector)

Where they also provide the following approximation for relatively large lattice potentials.

$$J \approx \frac{4}{\sqrt{\pi}} E_r \Big(\frac{V_0}{E_r}\Big)^{3/4} e^{-2\sqrt{V_0/E_r}} \tag{19}$$

Which is valied to within 10% for $V_0 > 15E_r$.

In the classic paper, Jaksch et al [3] provide the following approximation

$$U = \hbar\bar{\omega}\frac{a_s}{\bar{a_0}}/\sqrt{2\pi} \tag{20}$$

Where a_s is the scattering length, a_0 is the size of the ground state wavefunction, and the overbars indicate the geometric mean of the respective quantities. If we consider our lattice in such a configuration that each beam is operating at, say $30E_R$, then this expression produces $U = 4.27E^{-30}J = 0.311E_R$

In the 2006 review on BEC dynamics [6], we find a treatment of the limits of high and low optical potentials for the linear (non-interacting?) regime of a lattice-confined BEC. In particular, the tight-binding limit of the lowest energy band is

$$\begin{aligned} \frac{E(q)}{E_R} &= \sqrt{s} - 2J\cos(qd) \\ J &= \frac{4}{\sqrt{\pi}}(s)^{3/4}e^{-2\sqrt{s}} \\ s &= V_lat/E_R \end{aligned} \tag{21}$$

Note that this paper considers a potential of the form $V_{lat}\cos^2(kx)$, where $d = \lambda/2$ is the lattice periodicity. It seems that this J is the tight-binding approximation of the tunnelling energy, but this is unclear. In any case, the lattice amplitude is the same. In the case of our lattice this should be about $5.4E_r$ with a very weak dependence on q. That is, the atom is strongly confined to a particular lattice site.

In the weak-binding case, the result from Ashcroft and Mermin (1976) is quoted,

$$\frac{E(\bar{q})}{E_R} = \bar{q}^2 \pm \sqrt{4\bar{q}^2 + \frac{s^2}{16}} \tag{22}$$

Where $\bar{q} = q/k - 1, s = V_0/E_R$, and the plus (minus) sign provides the energy of the excited (ground) state, resp.

Also we finally caved and took out Ashcroft and Mermin on Solid State Physics [1]. They provide a wonderfully lucid proof of Bloch's theorem from symmetry considerations, and it has really brightened my day.

References

[1] Neil W. Ashcroft and N. David Mermin. *Solid State Physics*. Thomson Learning, 1976.

[2] Immanuel Bloch, Jean Dalibard, and Wilhelm Zwerger. "Many-Body physics with Ultracold Gases". In: *Reviews of Modern Physics* 80 (2008).

[3] D. Jaksch et al. "Cold bosonic atoms in optical lattices". In: *Physical Review Letters* 81 (1998).

[4] M. Machholm, C. J. Pethick, and H. Smith. "Band Structure, elementary excitations, and stability of a Bose-Einstein condensate in a periodic potential". In: *Physical Review A* 67 (2003).

[5] Harold J. Metcalf and Peter van der Straten. *Laser Cooling and Trapping*. Springer-Verlag, 1999.

[6] Oliver Morsch and Markus Oberthaler. "Dynamics of Bose-Einstein condensates in optical lattices". In: *Reviews of Modern Physics* 78 (2006).