Finite-curvature scaling in optical lattice systems

C. Hooley [a], J. Quintanilla [b,*],

[a] School of Physics and Astronomy, University of Birmingham, Edgbaston, Birmingham B15 2TT, U.K.
[b] ISIS facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire OX11 0QX, U.K.

Abstract

We address the problem posed by the inhomogeneous trapping fields when using ultracold fermions to simulate strongly correlated electrons. As a starting point, we calculate the density of states for a single atom. Using semiclassical arguments, we show that this can be made to evolve smoothly towards the desired limit by varying the curvature of the field profile. Implications for mutually interacting atoms in such potentials are briefly discussed.

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Since the first observation of Bose-Einstein condensation in a trapped gas of ultra-cold atoms [1], there has been an explosion of experimental and theoretical work on such systems. More recent developments include adding to the trapping fields a laser standing wave (a so-called 'optical lattice'). This generates an effective potential for the atoms which is given by

$$V(x) = V_0 \cos\left(\frac{2\pi x}{a}\right) + V_{\rm trap}(x), \qquad (1)$$

where a is the spatial period of the optical lattice, V_0 its strength, and $V_{\rm trap}(x)$ the effective potential due to the trapping fields. (The generalisation of (1) to more than one dimension is straightforward.) Recently, degenerate fermions have been loaded into such optical lattices [2], opening up the possibility of simulating strongly correlated electrons. Here we explore this prospect by considering, as a starting point, the single-atom density of states (DOS).

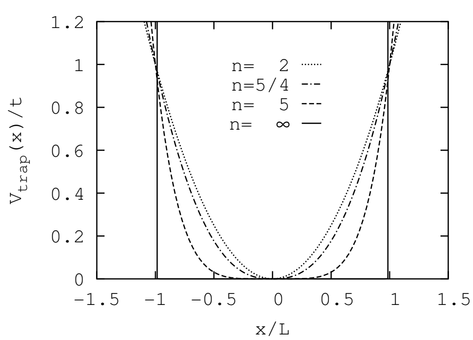

Fig. 1. Confining potential for various values of n, as indicated.

Perhaps the simplest case is that in which the optical lattice is very strong. In this case, we can replace the full Hamiltonian,

$$H_{\rm full} = \frac{\hat{p}^2}{2m} + V_0 \cos\left(\frac{2\pi x}{a}\right) + V_{\rm trap}(x), \qquad (2)$$

by a tight-binding version,

$$H = \sum_j \Big\{ -t\,|j\rangle\langle j+1| - t\,|j+1\rangle\langle j| + V_{\rm trap}(ja)\,|j\rangle\langle j| \Big\}, \qquad (3)$$

where $|j\rangle$ is a state in which the atom is in its local ground state on site j of the lattice.

In models of electron systems, one usually assumes the confining potential to be a 'box': $V_{\rm trap}(x) = 0$ for $|x| < L$, ∞ otherwise (the solid line of Fig. 1). In the bulk limit,

$$L \to \infty, \qquad (4)$$

$V_{\rm trap}(x)$ vanishes everywhere and one obtains the usual tight-binding DOS (the solid line of Fig. 2).

On the other hand, ultracold atoms are usually subject to a harmonic trap: $V_{\rm trap}(x) = t(x/L)^2$. The bulk limit (4) corresponds again to a vanishingly weak trapping potential, yet the DOS is qualitatively different. It is given by the dotted line in Fig. 2, as can be shown either via a WKB approach [3] or a 'local-density approximation' (LDA):

$$\rho(\epsilon) = \sum_j \rho_{\rm hom}(\epsilon - V_{\rm trap}(ja)), \qquad (5)$$

where $\rho_{\rm hom}(\epsilon)$ is the homogeneous DOS shown in Fig. 1. (We prove elsewhere that these two methods are equivalent.)

* Corresponding author. Tel: +44 (0)123 544 6353 Fax: 5720
Email addresses: c.hooley@bham.ac.uk (C. Hooley), j.quintanilla@rl.ac.uk (J. Quintanilla).

This state of affairs is unsatisfactory, in the sense that one would like to be able to interpolate smoothly between the harmonic scenario realised in atom-traps and the open boundary conditions of usual solid-state physics — particularly if one hopes to use the former to simulate the latter. We propose to achieve this by varying the form of the power law at $x = 0$. Consider the family of potentials

$$V_{\rm trap}(x) = t\left|\frac{x}{L}\right|^n . \qquad (6)$$

These reduce to the two cases studied above for $n \to \infty$ and $n = 2$, respectively. Let us therefore study the behaviour of the single-atom DOS of (3), with trapping potential (6), as a function of n. We call this progression through the family (6) 'finite-curvature scaling', by analogy with the finite-size scaling procedure used in numerical simulations [5].

We may obtain some information via straightforward asymptotics. Firstly, in the case $\epsilon \gg 2t$, we may neglect the first two terms in (3). What remains is just the $V_{\rm trap}$ term, the eigenstates of which are clearly the position eigenstates $|j\rangle$. The 'dispersion relation' is then $\epsilon = t|x/L|^n$, implying that $|x| = L(\epsilon/t)^{1/n}$, from which the DOS may readily be obtained:

$$\rho(\epsilon) \equiv \frac{dn}{d\epsilon} = \frac{dn/d|x|}{d\epsilon/d|x|} = \frac{2}{a}\frac{d|x|}{d\epsilon} = \frac{2L}{atn}\left(\frac{\epsilon}{t}\right)^{(1/n)-1} . \qquad (7)$$

This gives $\epsilon^{-1/2}$ behaviour in the harmonic case [3] in agreement with recent experiments [4]. Note that it also predicts ϵ^{-1} behaviour in the $n \to \infty$ limit; this prediction, though correct, is irrelevant, because the spectral weight at $\epsilon > 2t$ goes to zero as $n \to \infty$.

Secondly, we may look at the case $\epsilon \approx -2t$: these are the states very near the bottom of the band. For them, the tight-binding form of the DOS can be expanded around $k = 0$: $\epsilon_{\rm hom}(k) = -2t\cos(ka) \approx -2t + ta^2k^2$, corresponding to the kinetic energy of a free particle with mass $m_{\rm eff} = \hbar^2/2ta^2$. The total energy (classically) would therefore be given by

$$\epsilon = -2t + p^2/2m_{\rm eff} + V_{\rm trap}(x); \qquad (8)$$

using this relation as the orbit equation, and applying the WKB approximation as in the harmonic case [3], one can show that the DOS near the bottom of the band has the form

$$\rho(\epsilon) \sim (\epsilon + 2t)^{(1/n)-(1/2)} . \qquad (9)$$

This produces the correct square-root singularity in the $n \to \infty$ limit, and the previously calculated constant behaviour in the harmonic trapping case. Notice that, according to (9), a singularity exists at the bottom of the band for any $n > 2$.

To explore what happens at the top of the band ($\epsilon \sim 2t$), we evaluate the DOS in the LDA approximation (5) numerically. The results for a few different values of n are shown in Fig. 2.

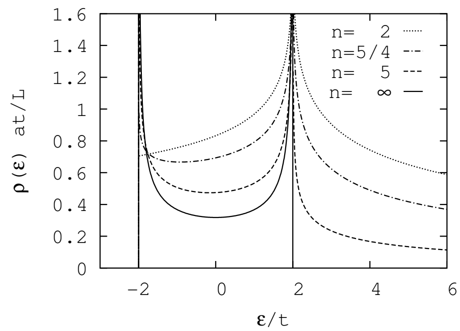

Fig. 2. The density of states for various values of n, as indicated. As n increases, the singularity at $\epsilon = -2t$ strengthens, while the one at $\epsilon = 2t$ becomes increasingly asymmetric.

In summary, we have presented an examination of the DOS of a single atom in a strong optical lattice plus a shallow power-law confining potential. Varying the power law permits one to scale from the case of harmonic trapping to the hard-wall case relevant to solid-state physics, and we call this variation finite-curvature scaling. The next step, for fairly weakly interacting atoms, would be to introduce the atom-atom interactions perturbatively. In the fermionic case, one can see that something special will happen (enhanced susceptibilities, or perhaps even ordering) when the chemical potential lies near the singularity at $\epsilon = 2t$. Analysis of this case is the subject of current research.

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