Quantum Capillary Waves at the Superfluid–Mott Insulator Interface

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We discuss quantum fluctuations of the interface between a superfluid and a Mott-insulating state of ultracold atoms in a trap. The fluctuations of the boundary are due to a new type of surface modes, whose spectrum is similar—but not identical—to classical capillary waves. The corresponding quantum capillary length sets the scale for the penetration of the superfluid into the Mott-insulating regime by the proximity effect and may be on the order of several lattice spacings. It determines the typical magnitude of the interface width due to quantum fluctuations, which may be inferred from single site imaging of ultracold atoms in an optical lattice.

PACS numbers: 64.70.Tg, 67.10.Jn, 67.80.bf, 67.85.Hj

The study of fluctuating interfaces is one of the central topics in statistical physics [1], with implications for phenomena like wetting or capillary forces [2] or the physics of biological membranes [3]. The origin of interface fluctuations in these cases is purely thermal. In recent years, a lot of interest has focussed on phase transitions that are driven by quantum rather than thermal fluctuations [4]. Somewhat surprisingly, the issue of interface fluctuations at the boundary between ground states with different order has not received much attention so far. In our present work, we study the interface between a superfluid (SF) and a Mott-insulator (MI) realized for ultracold bosons in an optical lattice [5] as an elementary example of a quantum interface problem. Since the MI-SF transition is of second order, the coexistence of ground states with different order in this case is due to the presence of a trapping potential, which gives rise to a wedding cake structure of successive superfluid and Mott-insulating domains [6]. This nontrivial spatial structure has been observed in a direct manner recently by a quantum gas microscope [7, 8], which provides single site resolution of individual atoms in an optical lattice. Within the standard local density approximation (LDA), the SF-MI interface is sharp. Specifically, for a 2D gas in an isotropic trap, it is a perfect circular line. Its position is determined by the condition that the local value of the chemical potential is equal to the critical value for the generic, density driven SF-MI transition of the homogeneous system [9] (see Fig. 1). As we will show below, a calculation which incorporates fluctuations around a spatially varying smooth background profile of the superfluid order parameter near the SF-MI boundary gives rise to fluctuations of this interface. They lead to a quantum uncertainty in its position which can be described in terms of an effective capillary length $\lambda_g$. The spectrum $\omega(k)$ of the elementary excitations, which are localized near the interface, crosses over from a gravity wave like form $\omega(k) = \sqrt{g_{eff}k}$ at small wave numbers $k\lambda_g \ll 1$ to a free particle like dispersion $\omega(k) \sim k^2$ at $k\lambda_g \gg 1$. This is reminiscent of classical capillary waves, where the role of gravity is played by the external trap potential. The $k^2$ behavior at short wavelengths is due to the fact that the SF order parameter vanishes exponentially as one moves into the MI region. Interactions between the mobile particles thus become negligible. The resulting free particle dispersion is quite different from the $k^{3/2}$ behavior found for standard capillary waves, which is due to a non-zero surface tension. In the SF-MI case, the latter is zero, however, because the transition is continuous [4, 9]. An important feature of this spectrum is that the amplitude of quantum fluctuations of the position of the SF-MI boundary diverges as the density gradient goes to zero. On the qualitative level mentioned above, the waves are similar to crystallization waves at the rough superfluid-crystal boundary of $^4$He [10]. However, there are important differences between these cases. The superfluid-crystal transition in $^4$He is of first order, with a jump of the density at the boundary. As a result the crystallization wave spectrum has a form $\omega \sim k^{3/2}$, and quantum fluctuations of the boundary position do not diverge. Moreover, recent experiments indicate that the superfluid-crystal boundary of $^4$He is quantum smooth and that crystallization waves occur only at finite temperature [11].

For a quantitative description of interface fluctuations, we use an effective action approach, with $\phi(x, \tau)$ the complex scalar order parameter of the superfluid [9]. At the mean field level, the SF-MI transition appears when the dimensionless coefficient $r$ of the quadratic contribution $r|\phi|^2$ to the effective Lagrange density vanishes. In the presence of the trap, $r(x)$ is spatially dependent, vanishing at a sharp boundary within LDA. Choosing a coordinate system where this boundary coincides with the $y$-axis, we have $r = bx + \ldots$ locally. The coefficient $b$ is determined by the associated gradient of the chemical potential $\mu$. Since all other coefficients of the effective action $S[\phi]$ for the order parameter are finite near this boundary, the relevant model to describe interface fluc-
FIG. 1: Qualitative zero temperature phase diagram of the homogeneous Bose-Hubbard model. In a trap, the local value of the chemical potential varies from a maximum in the center to the value where the density vanishes (vertical line). A SF MI interface appears in the vicinity of a generic transition point (marked with black dots). Specifically, we will discuss the transition on the lower side of the Mott lobe marked by the heavy dot.

Fluctuations near the SF-MI transition is given by

\[ S[\phi] = \int d^2x d\tau \left\{ \xi_0^2 |\nabla \phi(x, \tau)|^2 + bx|\phi(x, \tau)|^2 + u|\phi(x, \tau)|^4 + d\phi^*(x, \tau)\partial_\tau \phi(x, \tau) \right\}. \]  

(1)

Quite generally, the coefficients \( \xi_0, b, u \) and \( d \) are phenomenological parameters. Within a Bose-Hubbard model description of the SF-MI transition, they can be calculated directly from the hopping and interaction energy parameters \( J \) and \( U \) of the microscopic Hamiltonian, using the dimensionless function \( \xi = \frac{\xi_0}{\sqrt{\tau}} \) in a homogeneous system, diverging as \( (\mu - \mu_c)^{-1/2} \) at the transition. Note that we are considering the problem in two dimensions, which is the upper critical dimension since the dynamical exponent is \( z = 2 \) for the generic SF-MI transition [11, 9]. As a result, mean field theory correctly describes the divergence of the correlation length up to logarithmic corrections. In the presence of an external trap potential, the coefficient \( r \) vanishes linearly in the vicinity of the sharp SF-MI interface that results within LDA. The characteristic length scale \( \lambda_g \) over which this sharp profile will be smeared out by fluctuations is determined by the condition \( \xi_0/\sqrt{\tau(\lambda_g)} = \lambda_g \). It identifies \( \lambda_g \) with the scale at which the local correlation length reaches \( \lambda_g \) itself [14]. This results in a broadening of the interface over a scale \( \lambda_g = (\xi_0^2/b)^{1/3} \), a result that is borne out in detail by our calculation below.

The equilibrium order parameter profile can be obtained by solving the Euler-Lagrange equation corresponding to the action which reads

\[ \ddot{\phi}^\prime - \tilde{\phi} - |\tilde{\phi}|^2 \tilde{\phi} = 0, \]  

(3)

where we have defined \( z = x/\lambda_g \) and \( \tilde{\phi} = \phi/\phi_0 \) with \( \phi_0 = \sqrt{b\lambda_g/2a} \). This equation does not have a closed-form solution, but one readily finds the asymptotic behavior, i.e., \( \phi \sim \sqrt{-z} \) for \( -z \gg 1 \). For \( z \gg 1 \), the nonlinear term becomes negligible and Eq. (3) becomes the Airy differential equation which is solved by \( \phi = \text{Ai}(z) \). For arbitrary \( z \), the solution can be obtained numerically. The resulting order parameter profile \( n_k^{(0)}(z) = |\tilde{\phi}|^2 \) is shown in Fig. 2 and is formally identical to that obtained at a SF-vacuum boundary [15–17]. Note however that in the present case the characteristic length \( \lambda_g \) is different. In particular, it depends explicitly on the interactions \( g \), considering the problem in two dimensions, which is the upper critical dimension since the dynamical exponent is \( z = 2 \) for the generic SF-MI transition [11, 9]. As a result, mean field theory correctly describes the divergence of the correlation length up to logarithmic corrections. In the presence of an external trap potential, the coefficient \( r \) vanishes linearly in the vicinity of the sharp SF-MI interface that results within LDA. The characteristic length scale \( \lambda_g \) over which this sharp profile will be smeared out by fluctuations is determined by the condition \( \xi_0/\sqrt{\tau(\lambda_g)} = \lambda_g \). It identifies \( \lambda_g \) with the scale at which the local correlation length reaches \( \lambda_g \) itself [14]. This results in a broadening of the interface over a scale \( \lambda_g = (\xi_0^2/b)^{1/3} \), a result that is borne out in detail by our calculation below.

In the following, we consider quantum fluctuations around this mean field order parameter profile. To this end, we expand the action (1) second order in deviations from the mean field solution \( \phi_0 \). When \( \phi_0 \) is small, it is natural to consider fluctuations of the real and imaginary part of \( \phi \), i.e., \( \phi = \phi_0 + \varphi + i\psi \). Conversely, where \( \phi_0 \) takes appreciable values it is more natural to take into account the \( U(1) \) symmetry of the action and consider fluctuations of \( n_\sigma \) and \( \theta \), where \( \phi = \sqrt{n_\sigma e^{i\theta}} \). In both cases, fluctuations take on the form of plane waves parallel to the interface while in the direction perpendicular to the interface they form a set of modes which must be determined from a solution of the Euler-Lagrange equations. The equations for the dimensionless versions of \( \varphi \) and \( \psi \) (for ease of notation, we omit the tilde in the following) read

\[ \varphi'' - (z + 3n_\sigma^{(0)} + k^2)\varphi + i\omega \psi = 0 \]

\[ \psi'' - (z + n_\sigma^{(0)} + k^2)\psi - i\omega \varphi = 0, \]  

(4)
with \( n_{a}^{(0)} = \phi_{0}^{2} \). In the density-phase representation it is convenient to define \( T = \phi_{0} \theta \) and \( N = \delta n_{a}/\phi_{0} \) which obey the coupled equations

\[
\begin{align*}
T'' - (f + k^{2})T - i\omega N &= 0, \\
N'' - (f + 2n_{a}^{(0)} + k^{2})N + i\omega T &= 0,
\end{align*}
\]

where \( f = \partial_{z}^{2}n_{a}^{(0)}/2n_{a}^{(0)} - (\partial_{z}n_{a}^{(0)}/2n_{a}^{(0)})^{2} \). Asymptotically, \( f \sim z \) for \( z \gg 1 \) and \( f \sim -1/4z^{2} \) for \( -z \gg 1 \). The function \( f(z) \) is shown in Fig. 2.

The asymptotic behavior for small and large \( \omega \) is characterized by the integer \( n \), each branch having a gravity wave like \( \sqrt{k} \) dispersion. To make this analogy more explicit, one may write the lowest branch as \( \omega = \sqrt{g_{\text{eff}}k} \), with \( g_{\text{eff}} = 2g_{0}^{2}/d^{2} \). An equivalent dispersion relation has been derived in the context of the boundary of a dilute Bose-Einstein condensate in [19].

![Fig. 2: The mean field superfluid density \( n_{a}^{(0)} \) and the function \( f \) appearing in the differential equations for \( T \) and \( N \) as functions of \( z \), in dimensionless units.](image)

![Fig. 3: The two lowest branches of the dispersion relation \( \omega(k) \) as obtained from a numerical calculation (solid lines). The asymptotic behavior for small and large \( k \) is indicated with dotted lines.](image)
equations in the context of the boundary of a dilute BEC, where the lowest band dispersion was derived using a finite difference method \([21]\). The crossover in the lowest band indeed happens at \(k \lambda_g \approx 1\) so that \(\lambda_g\) plays a role analogous to that of the capillary length in the physics of surface waves on deep water. Note that this is completely different from the results of a previous analysis of boundary fluctuations of the SF-MI interface by Mariani and Stern [22], who found a large \(k\) scaling \(\omega(k) \sim k^{3/2}\) based on a model with a phenomenological nonzero surface tension.

To estimate the spatial extension of the fluctuation region, we introduce the phenomenological height variable \(h(y,t) = \lambda_g \delta n(y,0,t)/\partial_2 n_s^{(0)}\). The mean square fluctuations \(\langle h^2 \rangle\) would diverge if there was only the \(k^2\) part of the dispersion, and are made finite due to the crossover to gravity waves \(\omega \sim \sqrt{k}\) precisely as in the case of classical capillary waves. In the long wavelength regime, the action can be parametrized using the modes [6] and then reads

\[
S = \frac{\beta \xi_0^2 d}{2\mu} \sum_{k,m,n} \left( \frac{\omega_n^2}{\omega_m^2} - 2 \right) \left( \frac{\theta_{k,m,-n}}{\delta n_{k,m,n}} \right),
\]

where \(\omega_n = 2\pi n/\beta \omega_g\) are the bosonic Matsubara frequencies, rendered dimensionless. Note that the combination \(\xi_0^2 d/\mu\) of the dimensionful Landau-Ginzburg coefficients is dimensionless. This representation allows to calculate the variances of \(\theta\) and \(\delta n\). A lower bound to the total fluctuations is then given by the contribution from the lowest branch and wavelengths smaller than \(\lambda_g\):

\[
\langle h^2 \rangle \gtrsim \langle h^2 \rangle_c = \frac{2\sqrt{2}}{5\pi} \frac{u}{\xi_0^2 d} \lambda_g^2
\]

i.e., the fluctuations are infrared convergent so that the fluctuation region remains confined to the mean field transition region and the interface is quantum smooth.

To estimate whether the predicted zero point fluctuations of the SF-MI interface may be observed with current experiments, we take the typical case of \(^{87}\)Rb atoms in an optical lattice of period \(l = 532\, \text{nm}\), a lattice height of \(V_0 = 16.4 E_r\) which is close to the transition point for the MI-SF transition at unit filling \(g = 1\) \((E_r = \hbar^2/2m\lambda_{g}\mu)\) is the recoil energy) and a central chemical potential \(\mu(0) = 1.1 \mu_e\). With these parameters, the effective capillary length \(\lambda_g\) is equal to one lattice spacing for an isotropic harmonic trap with frequency \(2\pi \times 16.3\, \text{Hz}\). Moreover, the characteristic frequency \(\omega_g = \sqrt{g_{\text{eff}}/\lambda_g}\) where the spectrum crosses over from a gravity-like form \(\sim \sqrt{k}\) to the free particle \(\sim k^2\) regime is about \(2\pi \times 9\, \text{Hz}\). To see quantum fluctuations of the interface requires the temperature to be smaller than \(\hbar \omega_g/k_B = 0.43\, \text{nK}\). This is quite challenging to reach but appears feasible with novel cooling techniques like spin gradient demagnetization, where temperatures around 0.35 nK have recently been achieved in a similar setup [23]. Note that the regime \(\hbar \omega_g > k_B T\) that is required to see quantum fluctuations of the interface is opposite to the standard semiclassical limit \(\hbar \omega \ll k_B T\) that is usually considered in the thermodynamics of trapped BECs [24]. Moreover, for the parameters above, the characteristic density at the transition is \(\phi_g^{12} \approx 0.125\) so that [multiplying by \(n_s^{(0)}(0)\)] the density of mobile holes in the transition region is about 0.034 per lattice site. Using a quantum gas microscope [21], the smooth non-LDA mean field profile can be measured by averaging over a sufficiently large number of images. To probe the dispersion relation, one needs to selectively excite individual modes which can equally be achieved thanks to the single-site addressability of quantum gas microscopes: by modulating, e.g., the lattice depth on the single-site level, one can achieve values of \(2\pi \sqrt{k}/R\) ranging from \(4\pi R\) (corresponding to the quadrupole mode, with \(R\) the radius of the LDA transition circle) down to \(2l\). Since \(\lambda_g\) can take any value from practically zero to several lattice sites, this permits to map out the crossover shown in Fig. [3]. With the stated parameters, the experimental detection of the interface’s quantum dynamics is certainly challenging, but within reach of current experimental technology. Additional flexibility may be gained from the use of nonharmonic potentials using phase plates. For example, a box-like potential with an added localized strong variation permits to have the transition happen at a larger radius so that more atoms participate.

In summary, we have discussed the zero temperature quantum fluctuations of the MI-SF interface and found that the associated dispersion relation leads to a quantum smooth surface. An experimental observation of these fluctuations requires very shallow trap potentials, where the associated capillary length \(\lambda_g \sim \omega^{-1/3}\) is at least several lattice spacings. From a more general point of view, the interface fluctuations we discussed here are just a particular case of the rich physics of interfaces in quantum phase transitions. For example, in recent years, a completely new type of interfaces has turned into the focus of research, in which novel phases appear at the boundary between two materials with different ground states. A striking example is the appearance of a conducting 2D electron gas and even tunable superconductivity at the boundary between two insulators [25].

We are grateful for helpful discussions with I. Bloch, F. Gerbier and M. Greiner. B. S. acknowledges financial support from the Humboldt foundation, S. P. R. and W. Z. from the DFG within the Forschergruppe 801.

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