计算物理

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Method

```
In[21]:= f1 = x + 0.5 * y - 1.0;
         f2 = x^2 + y^2 - 2.4;
         sol = Solve[{f1 == 0, f2 == 0}, {x, y}, Method → {"Newton", "StepControl" → "TrustRegion"}]

... Solve: Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a
    corresponding exact system and numericizing the result.

Out[23]= {{x → 0.234315, y → 1.53137}, {x → 1.36569, y → -0.731371}}

In[24]:= f1 /. sol[[1]]
         f2 /. sol[[1]]
         f1 /. sol[[2]]
         f2 /. sol[[2]]

Out[24]= 0.

Out[25]= 0.
```

Out[26]= 5.55112×10^{-17}

Out[27]= 1.11022×10^{-16}

```
F = f1 * f1 + f2 * f2;
FindMinimum[F, {x, 0}, {y, 0}, Method → {"Newton", "StepControl" → "TrustRegion"}]
```

$\{8.63089\times10^{-24}, \{x\to1.36569, y\to-0.731371\}\}$

```
NDSolve[{x''[t] + (2 + Sin[x[t]]) x[t] == 0, x[0] == 1, x'[0] == 0},
 x, {t, 0, 10}, Method → "ExplicitRungeKutta"]
```

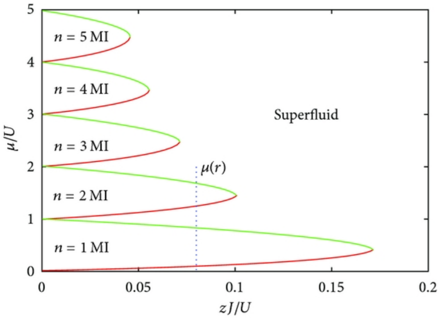
{{x → InterpolatingFunction[ Domain: {{0., 10.}} Output: scalar]}}

```
NDSolve[{x''[t] + Sin[x[t]] == 0, x[0] == 3, x'[0] == 0},
 x, {t, ∞}, Method → {"EventLocator", "Event" → x[t],
   "EventAction" :→ Throw[end = t, "StopIntegration"], Method → "BDF"}]
```

{{x → InterpolatingFunction[ Domain: {{0., 4.04}} Output: scalar]}}

最小值问题和求根问题在很多时候可以等价，但是它们在数值处理上可能有所不同．这两种方法各有所长．

Mott Phase

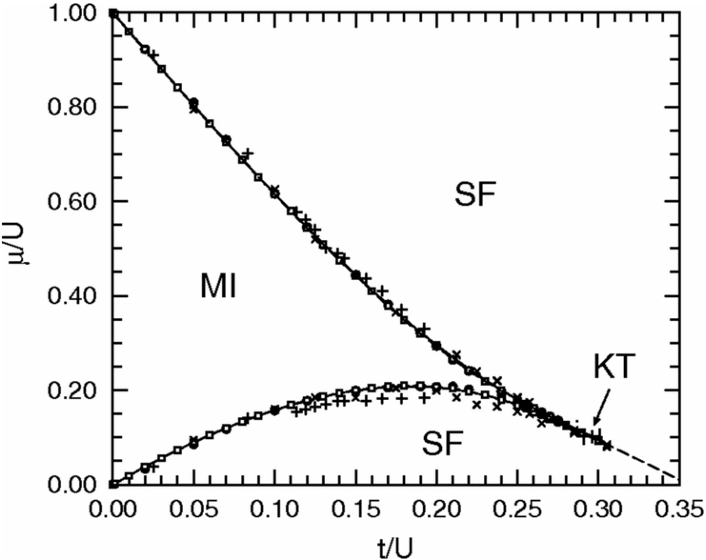


$$H = \sum_{i,j} -J c_i^\dagger c_j + \text{h.c.} + \sum_i \frac{U}{2} n_i(n_i - 1) - \mu n_i.$$

At $J = 0$,

$$\frac{U}{2} n(n-1) - \mu n = \frac{U}{2}(n+1)n - \mu(n+1) \to \mu = nU.$$

Mott Phase



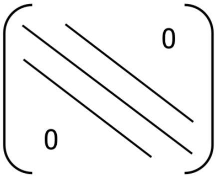
1.00
0.80
0.60
0.40
0.20
0.00
μ/U
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
t/U
SF
MI
KT
SF

平均场理论

$$\hat{H}_{\rm MF} = \sum_i -Jz(\psi^* \hat{a}_i + \psi \hat{a}_i^\dagger - |\psi|^2) + \frac{U}{2}\hat{n}_i(\hat{n}_i - 1) - \mu\hat{n}_i$$

Diagonalization in site-basis

$\hat{H}_{\rm MF} =$



K. Sheshardi et al., EPL 22, 257 (1993)

Perturbation Theory

$$\hat{H}_0 = Jz\psi^2 + \tfrac{U}{2}\hat{n}(\hat{n}-1) - \mu\hat{n}$$

$$\hat{V} = -Jz\psi(\hat{a} + \hat{a}^\dagger)$$

van Oosten et al., PRA 63, 053601 (2001)

Second-order perturbation theory:

$$E = E_0 + \langle n|V|n\rangle + \sum_{m\neq n}\frac{\langle m|V|n\rangle\langle n|V|m\rangle}{E_n - E_m}.$$

```
In[2]:= En =  J z ψ^2 + U n (n - 1) / 2 - μ n;
        Eplus = En /. {n → n + 1};
        Eminus = En /. {n → n - 1};
        Esecond = (J z ψ) ^2 (n + 1) / (Eplus - En) + (J z ψ) ^2 (n) / (Eminus - En)
```

Out[5]= $\frac{J^2 n z^2 \psi^2}{\frac{1}{2}(-2+n)(-1+n)U - \frac{1}{2}(-1+n)nU - (-1+n)\mu + n\mu} + \frac{J^2(1+n)z^2\psi^2}{-\frac{1}{2}(-1+n)nU + \frac{1}{2}n(1+n)U + n\mu - (1+n)\mu}$

```
In[8]:= F = FullSimplify[En + Esecond]
```

Out[8]= $\frac{1}{2}n((-1+n)U - 2\mu) - \frac{Jz(n^2U^2 + (U+\mu)(Jz+\mu) - nU(U+2\mu))\psi^2}{((-1+n)U-\mu)(nU-\mu)}$

```
In[10]:= FullSimplify[Coefficient[F, ψ^2]]
```

Out[10]= $Jz\left(1 + \frac{Jz(U+\mu)}{(nU-\mu)(U-nU+\mu)}\right)$

$$E(n+1) - E(n) = Un - \mu, \quad E(n-1) - E(n) = \mu - U(n-1).$$

$$\langle n|(a+a^\dagger)|n+1\rangle = \sqrt{n+1}, \quad \langle n|(a+a^\dagger)|n-1\rangle = \sqrt{n}.$$

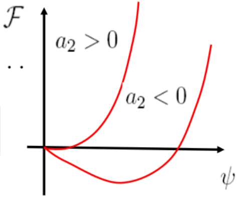
Thus for $F = F_0 + F_2$

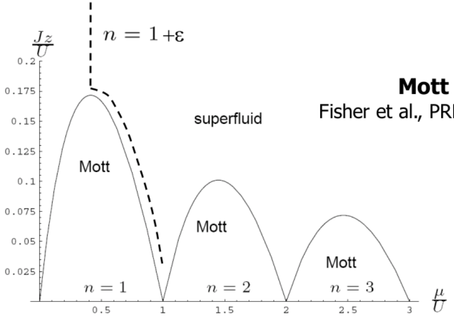
$$F_2 = Jz\psi^2 + (Jz\psi)^2\frac{n+1}{Un-\mu} + (Jz\psi)^2\frac{n}{\mu - U(n-1)} = ()\psi^2.$$

Landau 相变理论

$$\mathcal{F}(\psi^*, \psi) = a_0 + a_2|\psi|^2 + a_4|\psi|^4 + \ldots$$

$$a_2 = Jz + J^2 z^2 \frac{U+\mu}{(\mu - Un)[U(n-1)-\mu]} \stackrel{!}{=} 0$$



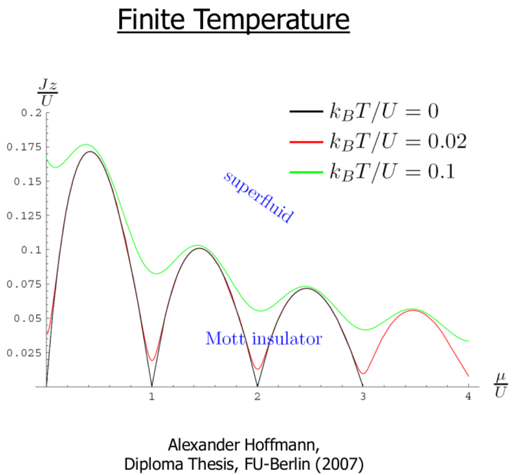


Mott Lobes

Fisher et al., PRB 40, 546 (1989)

Alexander Hoffmann,
Diploma Thesis, FU-Berlin (2006)

有限温度相图



From: Axel Pelster et al, Bose-Hubbard Model (BHM) at Finite Temperature.

有限温度相图

$$b_i^\dagger b_j = \langle b_i^\dagger \rangle b_j + \langle b_j^\dagger \rangle b_i - \langle b_i^\dagger \rangle \langle b_j^\dagger \rangle = \phi(b_i^\dagger + b_j) - \phi^2, \quad (2)$$

where $\phi = \langle b_i^\dagger \rangle = \langle b_i \rangle$ is the superfluid order parameter. The Hamiltonian of the Bose-Hubbard model can be written as a sum over single-site terms, $H = \Sigma_i H_i$, where

$$H_i = \frac{U}{2} n_i(n_i - 1) - \mu n_i - zt\phi(b_i^\dagger + b_i) + zt\phi^2, \quad (3)$$

with z being the number of nearest neighbors. In Ref. [10], Sheshardi *et al.* have studied the zero-temperature properties of the Bose-Hubbard model by diagonalizing the Hamiltonian H_i in the occupation number basis $\{|n\rangle\}$ truncated at a finite value n_t. Here, we will extend this method to include the temperature effects [23] and investigate the finite-temperature properties of the same model. We first obtain the matrix of H_i in the truncated occupation number basis, which has a symmetric tridiagonal form:

$$\begin{pmatrix} d(1) & e(1) & 0 & \dots & & & 0 \\ e(1) & d(2) & e(2) & & & & \vdots \\ 0 & e(2) & d(3) & & & & \\ \vdots & & & \vdots & & & \\ & & & & d(n_t-1) & e(n_t-1) & 0 \\ & & & & e(n_t-1) & d(n_t) & e(n_t) \\ 0 & \dots & & & 0 & e(n_t) & d(n_t+1) \end{pmatrix}, \quad (4)$$

FIG. 1. (Color online) The finite-temperature phase diagram of the Bose-Hubbard model in the $\mu/zt - U/zt$ plane. The temperature is increasing when evolving away from the zero-temperature Mott lobes. The temperature T/zt of each curve is listed in a column on the right side of the figure. The red curves with values 0.5, 0.6, and 0.7 on them indicate the crossover region for the first Mott lobe, and the blue ones with 1.1, 1.2, and 1.3 on them indicate the crossover for the second lobe.

$$Z = \sum_{k=1}^{n_t+1} e^{-\beta E_k}, \quad F = -\frac{1}{\beta} \ln Z. \quad (7)$$

For given U, t, μ, and T, the superfluid order parameter ϕ can be determined by minimizing the free energy, i.e.,

$$\left.\frac{\partial F}{\partial \phi}\right|_{U,t,\mu,T} = 0. \quad (8)$$

The region with nonzero ϕ is identified as the superfluid phase while the region with $\phi = 0$ as the Mott-insulator or normal-liquid phase. After determining ϕ, it is easy to calculate other physical quantities such as the superfluid density ρ_s and average density ρ with

$$\rho_s = \phi^2, \quad \rho = \langle n \rangle = \frac{\mathrm{Tr}(n e^{-\beta H})}{Z}. \quad (9)$$

We show our main results in Figs. 1–4. The finite-temperature phase diagrams are plotted in Fig. 1 in the $\mu/zt - U/zt$ plane. The different curves represent the phase boundaries between superfluid and normal liquid (or MI) at

From: Xiancong Lu and Yue Yu, Phys. Rev. A 74, 063615 (2006).