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Spin correlations and doublon production rate for fermionic atoms in modulated optical lattices

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We compute the integrated doublon production rate in response to a lattice modulation for two-component fermions in an optical lattice. We derive a general formula for the integrated intensity, valid in the presence of inhomogeneous potentials such as the trap, which gives the integrated intensity in terms of equal time correlation functions only. Such a formula is thus well suited for direct numerical calculations. We show that, in the limit of large repulsion for commensurate fillings, or for temperature ranges for which the hopping is incoherent, the integrated doublon spectrum is directly related to the nearest-neighbor spin-spin correlation function. We compute its temperature dependence in this regime using finite temperature quantum Monte Carlo calculation.

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Ultracold atom gases confined in an optical lattice provide a controlled realization of the Hubbard model [1,2] which plays a central role in the study of strongly correlated electron systems such as Mott transition, high- T_c superconductivity, and quantum magnetism. Despite intensive research the phase diagram of this model is still largely debated. Cold atoms, with the control of the interactions using a Feshbach resonance technique and the control of kinetic energy via lattice depth, allow us to probe such physics in detail.

In order to do so, the development of experimental probes to capture many-body quantum states is also an important issue. In connection with the Hubbard physics, measuring the antiferromagnetic (AFM) correlations is of prime importance. However, this is not an easy task. The AFM order can potentially be extracted from time-of-flight measurements via shot-noise measurement [3–5]. However, the measurement is far from trivial and also depends crucially on the direction of the magnetic order. Local addressing [6,7] is also a potential route but systems are for the moment quite small, and in addition such a technique is complicated to extend to three-dimensional systems. It is thus highly desirable to study other probes that can potentially give direct access to the magnetic correlations [8–14].

One probe which has proved to be very efficient and relatively simple to implement is the amplitude modulation of the optical lattice [15]. This probe, first used for bosonic systems with a measurement of the absorbed energy, gives direct access to the kinetic energy correlation functions [16–18]. For fermions the energy absorption rate (EAR) cannot be implemented accurately enough and a variant of this probe measuring the doublon production rate (DPR) has been proposed [19]. This DPR measurement in the linear response regime could be successfully implemented [20], and thus stimulates further studies of theoretical calculation of DPR spectra [21–26] and doublon dynamics [27–29].

In addition, it was shown [19] by a direct comparison of the two quantities, that the integrated intensity of the modulation does directly give access to the nearest-neighbor AFM correlations. Intuitively, for fermionic atoms, spin configurations of neighboring atoms are relevant to the spectra because of the Pauli exclusive principle: while the hopping is allowed for neighboring atom spins pointing in antiparallel,

it is blocked for ferromagnetically aligned spin configuration. This point, which allows one to use the modulation as a simple probe of magnetism, was explored further both theoretically and experimentally in the linear response regime at high temperatures [30].

In this paper, we further analyze the integrated intensity of the DPR. We consider potentially inhomogeneous systems, e.g., due to the presence of the trap. We show that the frequency integrated DPR can be fully expressed, within linear response, in terms of static correlations. Such correlations, contrarily to the original DPR response at fixed frequency, are well within the reach, without any need for analytical continuation, of powerful numerical methods such as quantum Monte Carlo (QMC) simulation, thus potentially allowing a very precise comparison of the integrated DPR and theoretical calculations. For the case when the filling is commensurate and the interactions are large compared to the kinetic energy, or when the hopping is incoherent due to the temperature, that the above formulas reduce, in agreement with the initial study of Ref. [19], to a measure of the nearest-neighbor AFM correlation functions. We obtain the temperature dependence of this quantity via a QMC simulation of the Heisenberg quantum spin model in a three-dimensional cubic lattice.

We consider two-component fermionic atoms strongly confined in an optical lattice. In the case of deep optical lattices, the physics is well described by the spin-1/2 fermionic Hubbard model $H_0 = H_K + H_U + H_p$, with

$$H_K = -J \sum_{\sigma=\uparrow,\downarrow} \sum_{\langle i,j \rangle} c_{i\sigma}^\dagger c_{j\sigma}, \quad (1)$$

$$H_U = U \sum_j n_{j\uparrow} n_{j\downarrow}, \quad (2)$$

$$H_p = \sum_j v_j (n_{j\uparrow} + n_{j\downarrow}), \quad (3)$$

where $c_{j\sigma}$ and $n_{j\sigma}$ are, respectively, an annihilation and number operator of a fermionic atom at a j th site. The on-site potential v_j (for example, corresponding to trap potential) generally breaks translational symmetry.

The parameters J and U are given as a function of an amplitude of a sinusoidal lattice potential, i.e., $V_{\text{op}}(\mathbf{r}) = V_0[\cos^2(\pi x/a) + \cos^2(\pi y/a) + \cos^2(\pi z/a)]$, where the

lattice constant is a . [1] The dynamical amplitude modulation defined on continuum space is represented in an effective lattice model as follows: $J \rightarrow J[1 + \delta J \cos(\omega t)]$ and $U \rightarrow U[1 + \delta U \cos(\omega t)]$ corresponding to $V_0 \rightarrow V_0 + \delta V \cos(\omega t)$ for the lattice depth.¹ Thus the perturbation Hamiltonian of the lattice modulation is given as $V(t) = (\delta J) \cos(\omega t) H_K + (\delta U) \cos(\omega t) H_U$, but here we use the alternative representation to simplify the problem [17] as $V(t) = (\delta U) \cos(\omega t) H_0 + \cos(\omega t) S$ with

$$S = (\delta F) H_K - (\delta U) H_p, \quad (4)$$

where $\delta F = \delta J - \delta U$ is a dimensionless perturbation parameter. Note that in the homogeneous case ($v_j = v$) the perturbation operator becomes the kinetic energy H_K .

In the linear response regime, the DPR per site can be defined as an increment of the doublon number time averaged over a single period $2\pi/\omega$,

$$P_D(\omega) = \frac{1}{\Omega} \frac{1}{2\pi/\omega} \int_t^{t+(2\pi/\omega)} dt' \frac{d}{dt'} N_D(t'), \quad (5)$$

where $N_D(t)$ is the number of created doublons and Ω is a total site number of the system. Note that as seen below, the time dependency in the right-hand side should cancel due to the single-period time average in the linear response region. The doublon number can also be written by the Hubbard interaction $N_D(t) = \langle H_U \rangle / U$, which is averaged by the density matrix $\rho(t) = e^{-H(t)/k_B T} / \text{Tr}[e^{-H(t)/k_B T}]$ for time-dependent Hamiltonian $H(t) = H_0 + V(t)$. Thus the doublon number is also expressed as

$$N_D(t) = \frac{E(t) - \langle H_K + H_p \rangle - \langle V(t) \rangle}{U}, \quad (6)$$

where $E(t) = \langle H(t) \rangle$ is a system energy. In the second-order perturbation theory with respect to the lattice modulation $V(t)$, all terms in Eq. (6) apart from the first one are found to generate only oscillatory terms whose contribution to the DPR spectrum disappears due to the time average in Eq. (5). Therefore one can rewrite Eq. (5) as follows:

$$P_D(\omega) = \frac{1}{\Omega} \frac{1}{2\pi/\omega} \int_t^{t+(2\pi/\omega)} dt' \frac{1}{U} \frac{d}{dt'} E(t'). \quad (7)$$

Interestingly, the equality means that the DPR is equivalent to the EAR in the second-order response regime, as was pointed out in Ref. [19]. The EAR (7) as a second-order response can be formulated by the linear response theory. As a result, the DPR formula can be given [19] as

$$P_D(\omega) = -\frac{1}{\Omega} \frac{1}{2\hbar U} \text{Im}[\omega \tilde{\chi}_S^R(\omega)], \quad (8)$$

where $\tilde{\chi}_S^R(\omega) = -i \int_0^\infty dt e^{i\omega t} \langle [S(t), S(0)] \rangle_0$ is the Fourier transform of the retarded correlation function of the operator S for the unperturbed Hamiltonian H_0 .

We now consider the general formula of DPR spectra (8) integrated over the modulation frequency ω . Before implementing the integral, we clarify the point of the integral range of modulation frequency from an experimental point of view. In actual experiments a high-frequency cutoff is necessary. In order to discuss the needed cutoff, let us recall the setup of the Hubbard model. Atoms in an optical lattice form a Bloch band structure, and the band gaps are determined by the depth of the optical lattice potential. Since the single-band Hubbard model H_0 is introduced to demonstrate the physics in the lowest Bloch band, the high-energy cutoff necessary to justify the effective model should be taken to be sufficiently small compared with the band gap between the lowest and the next Bloch band. Therefore, by integrating the DPR spectrum over the frequency region below the band gap, the integration discussed below can be estimated in experiments.

The integrated DPR (8) reads

$$\int_0^\infty d\omega \omega \tilde{\chi}_S^R(\omega) = -\frac{1}{\hbar} \int_0^\infty dt \frac{\langle [[H_0, S(t)], S(0)] \rangle_0}{t + i0^+}. \quad (9)$$

Here the quantity $\langle [[H_0, S(t)], S(0)] \rangle_0$ in Eq. (9) is real. Thus the imaginary part in the right-hand side of Eq. (9) is caused by the denominator of the integrand. Using the decomposition $1/(t + i0^+) = \mathcal{P} \frac{1}{t} - i\pi \delta(t)$, where \mathcal{P} denotes the principal value, one can take the imaginary part, and obtain the dimensionless total spectrum weight Γ as

$$\Gamma \equiv \int_0^\infty \frac{d\omega}{(J/\hbar)^2} P_D(\omega) = -\frac{1}{\Omega} \frac{\pi \langle [[H_0, S], S] \rangle_0}{2J^2 U}. \quad (10)$$

This formula is one of the central results of this paper. Remarkably, Eq. (10) is deduced from Eq. (8) without any approximation, and in addition the inhomogeneity effect of the system is fully taken into account in the formula. It relates a dynamical quantity to a calculation of equilibrium correlation functions. Such correlations are easily amenable to a computation via a large number of numerical techniques such as QMC simulations, allowing us to make direct contact between the measured DPR spectrum and various quantities of the Hubbard model. One can thus, by comparing the experimental and theoretical results, expect to determine hard to get parameters, such as the temperature (or entropy).

Furthermore, as we will show below this general correlation, the generic formula (10) is reduced in the interesting regime of temperatures $k_B T \ll U$ to a direct measure of the spin-spin correlations. Equation (10) contains two-particle correlation functions such as $\langle c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger c_{k\uparrow} c_{l\downarrow} \rangle_0$. Thus the practical calculation is not trivial in general, and the physical interpretation is not also clear. In what follows, we separately consider the two limited but interesting regions: (i) high-temperature $k_B T \gg J$ and (ii) strongly correlated regime $J \ll U$ at half-filling. Note that the two-particle correlation functions can then be written as

$$\begin{aligned} \langle c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger c_{k\uparrow} c_{l\downarrow} \rangle_0 &= \delta_{i,k} \delta_{j,l} \langle c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger c_{i\uparrow} c_{j\downarrow} \rangle_0 \\ &+ \delta_{i,l} \delta_{j,k} \langle c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger c_{j\uparrow} c_{i\downarrow} \rangle_0. \end{aligned} \quad (11)$$

In the first case (i), hopping is incoherent regardless of the filling. Thus we can simply apply Eq. (11) to the generic

¹The second-order variations of J and U by the modulation δV can be taken into account as well, and do not affect the results on the EAR and DPR given in this paper.

formula (10). Consequently Γ simplifies as

$$\Gamma = -\frac{2\pi(\delta F)^2}{\Omega} \left[\bar{N}_D + \frac{1}{z} \sum_{(i,j)} \left(\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle_0 - \frac{\langle n_i^c n_j^c \rangle_0}{4} \right) \right] - \frac{\pi(\delta F)(\delta J)}{2\Omega} \sum_{(i,j)} \frac{v_i - v_j}{U} (\langle n_i^c \rangle_0 - \langle n_j^c \rangle_0), \quad (12)$$

where $n_j^c = \sum_{\sigma} n_{j\sigma}$, and z is a coordination number. The total doublon number in equilibrium state, $\bar{N}_D = \sum_j \langle n_{j\uparrow} n_{j\downarrow} \rangle_0$, has also been introduced. Note that the inhomogeneity of a system is also fully taken into account in formula (12). In the homogeneous case, since $v_i - v_j = 0$, Γ turns out to be given only by the first line.

In the second strongly interacting regime (ii), which allows us to reach much lower temperatures, one has to restrict the study to the half-filling homogeneous case to avoid regions in which coherent hopping could still exist. In particular, in the presence of a trap, this will occur in the shell of the compressible region. Hopefully such regions would give small contributions compared to the bulk of the response. In addition, the response of these regions is mostly concentrated at low energy rather than for energy or order U , and thus most of their contribution can be filtered away in the frequency integration. If we restrict to the commensurate case, the simplification (11) is still applicable for $k_B T \ll U$. Then the on-site potential term H_p essentially disappears,² and the integrated spectrum Γ turns out to be Eq. (10) in which S is replaced by $(\delta F)H_K$. The resultant Γ after applying Eq. (11) is given by the first line of Eq. (12). However, the density fluctuation would then be strongly suppressed, and one can approximately take $\bar{N}_D \approx 0$ and $\langle n_i^c n_j^c \rangle_0 \approx 1$, whose temperature dependency would be negligibly small. Therefore, the integrated DPR spectrum is given as

$$\Gamma = 2\pi z (\delta F)^2 \left[\frac{1}{4} - \frac{1}{z\Omega} \sum_{(i,j)} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle \right], \quad (13)$$

where z is a coordination number. What is important is that only the nearest-neighbor spin-correlation function $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ is a dominant contribution to the temperature dependence of Γ . Namely, Γ can be identical to the nearest-neighbor spin correlation.

The nearest-neighbor spin correlation appearing in Eq. (13) is exactly the same as the energy of the quantum spin Heisenberg model. As is well known, in the strongly interacting region $k_B T, J \ll U$, at half-filling, the Heisenberg model is deduced from the Hubbard model as a consequence of the second-order perturbation theory in terms of J/U . Thus, in such a region, Eq. (13) allows us to probe the system energy.

In order to see the temperature dependence of Γ , we numerically estimate the temperature dependence of the integrated DPR spectrum Γ . However, it is a highly nontrivial problem because it is necessary to compute the dynamical quantity (8) directly in a wide regime of temperature. Thus, in this paper

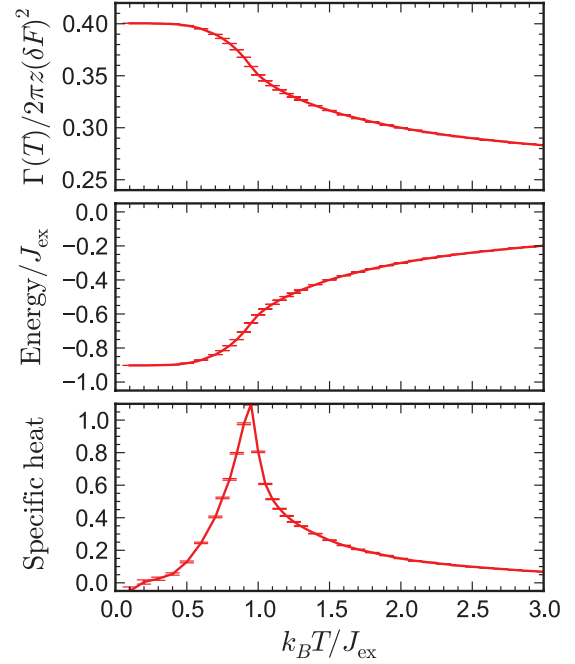


FIG. 1. (Color online) The temperature dependence of (top) the integrated DPR spectrum per site Γ scaled by $2\pi z(\delta F)^2$, (middle) the energy per site scaled by a superexchange spin coupling J_{ex} , which is identical to the nearest-neighbor spin correlation per site multiplied by the coordination number $z = 6$ in a cubic lattice, and (bottom) the specific heat. The QMC calculation is implemented for the quantities in the Heisenberg model for 14^3 system size. While error bars are also shown, they are negligibly small. The Néel transition occurs near $k_B T \approx J_{\text{ex}}$, and then the integrated spectrum and the energy per site exhibit an inflection-point-like behavior.

the parameter region is restricted to the regime for which the approximation (13) is valid, i.e., $k_B T, J \ll U$. In addition, we calculate the static quantity (nearest-neighbor spin correlation) $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ instead of integrating the DPR spectrum over the modulation frequency. In the low-temperature Mott insulating case, we can approximately choose the AFM Heisenberg model as an effective model, which allows one to compute the nearest-neighbor spin correlation through the energy of the Heisenberg model.

We implement the QMC calculation for the AFM Heisenberg model of a cubic lattice where the system size is $\Omega = 14^3$.³ The result is shown in Fig. 1, where the calculated energy is translated into Γ by use of the relation (13). As a reference of the critical temperature of the Néel transition [31,32], the specific heat as a function of temperature is also shown. The derivative of Γ as temperature rises is found to be maximum near the critical point, which seems an inflection point. On the other hand, the nearest-neighbor spin correlation and the energy for temperatures higher than the critical point exhibit long tail decay.

To summarize, we have explicitly discussed the DPR spectra in the presence of an inhomogeneous potential, and

²It is easily found that the result (13) in this discussion does not change, even if we leave H_p in the form of a homogeneous potential $v_j = v$.

³The calculations for $\Omega = 12^3$ and 10^3 have also been implemented, but no crucial difference has been found on the curves, showing that finite size corrections are already very small.

the generalized form of the DPR spectrum as a function of lattice modulation frequency has been obtained. In addition we have implemented the integration of the DPR spectrum over modulation frequency. The problem of dynamics can be reduced to the calculation of static quantity as shown in Eq. (10). Such a formula can be the basis of a very accurate numerical comparison with the experiment. Furthermore, focusing on the two different regimes, (i) $k_B T \gg J$ and (ii) $J \ll U$, a generic form of the integrated DPR spectrum has been deduced. In particular, for the incompressible Mott regime, it is found to be associated with the nearest-neighbor

spin correlation as in Eq. (13), and can thus be used as a probe of the magnetic properties. In the larger J regime, higher order hopping processes would be more relevant, and the integrated DPR spectrum is expected to probe longer-range spin correlations. One can thus use the shaking of the lattice and DPR to directly probe for magnetic order.

The calculation for temperature dependence of the energy has been implemented by using the looper QMC code of the ALPS libraries [33–38]. This work was supported by the Swiss National Foundation under MaNEP and division II.

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