Effect of Electron Correlation on the Bragg Reflection

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We study the effect of correlation on the Bragg reflection in the 3D electron gas, the 1D Luttinger liquid, and the 1D Hubbard model in an alternating periodic potential at half-filling. In the last system, we suggest a Luttinger-liquid-type quasi-metallic state in the crossover region from the band insulator to the Mott insulator. We explain the appearance of this state in terms of the incompatibility of the Bragg reflection with the concept of Luttinger liquids.

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One of the fundamental issues in solid state physics is to elucidate to what extent the concept of "electronic band structure" is relevant in a strongly-correlated system. In the free-electron gas, the band gap is formed by the quantum interference between an incident electron plane wave, $e^{i\mathbf{k}\cdot\mathbf{r}}$, with a reflected one, $e^{i(\mathbf{k}+\mathbf{K})\cdot\mathbf{r}}$, where $\mathbf{K}$ is a reciprocal-lattice vector related to periodicity of V an electron-lattice potential. In this sense, the quantum coherence leading to the Bragg reflection is a key to the band structure and thus we consider it quite important to study the correlation effect on the Bragg reflection.

The study is conceptually simple in the Fermi liquid as represented by the three-dimensional electron gas (3DEG) at metallic densities. The point is that we should grasp the band-gap formation in terms of the Bragg reflection of a quasi-particle rather than a free electron, because quasi-particles or wave packets composed of a complicated combination of plane waves due to U the electron-electron interaction manifest themselves in low-energy physics. In the one-dimensional Luttinger liquid (1DLL), however, the situation is not so simple [1]; we should ask even the very existence of the Bragg reflection and this constitutes one of the aims of this paper.

Basically there exist two complementary approaches to the many-electron system in a crystal described by the Hamiltonian H composed of T the kinetic energy, V, and U. One is "the band approach" or $(T+V)+U$ in which the problem is reduced to the self-consistent determination of an effective one-body potential $\widetilde{V}$ by combining V with the effect of U in the Hartree-Fock-like mean-field approximation. If desired, the correlation effect due to U (which is missed in $\widetilde{V}$) can be included by perturbation in U with respect to the unpertubed part $T+\widetilde{V}$. Another is "the correlated-electron approach" or $(T+U)+V$ in which we consider a correlated-electron state defined by $T+U$ first and then include V perturbatively. Note that these two approaches do not always provide the same conclusion, as the discussion on the Mott transition [2] indicates. We can even imagine situations in which the competition between V and U brings about a state which neither approach describes well.

In this paper, an example of such intriguing situations is shown on the basis of our finding that the Bragg reflection is usually incompatible with the concept of Luttinger liquids. More specifically we shall treat the 1D Hubbard model with an alternating periodic potential at half-filling, a system attracting much attention in relation to the neutral-ionic transition [3], the ferroelectric perovskites [4,5], and the crossover from the band insulator (BI) at $V \gg U$ to the Mott insulator (MI) at $V \ll U$ [6–8]. We have made a study in the density-matrix renormalization group (DMRG) [9] to obtain the charge and spin gaps, Δ_c and Δ_s, as well as the electron localization length λ with the system size up to 400 sites (which is larger than any previous calculations by an order of magnitude). By comparing these exact results with approximate ones given in both the band and correlated-electron approaches and also by referring to the very recent result of Fabrizio *et al.* [10], we suggest the appearance of a Luttinger-liquid-type quasi-metallic state at the BI-MI crossover. Here by "quasi-metallic" we mean that it is not the same as "metallic" because of nonzero Δ_c, but the state is distinct from either BI or MI by such features as very small Δ_c and long λ.

For better illustration of the Bragg reflection of a quasi-particle, let us start with 3DEG in a weak periodic potential V for which H is given in second quantization with the plane-wave basis as [11]

$$H = T+V+U = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c^{+}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{K}\neq\mathbf{0}} \sum_{\mathbf{k}\sigma} V(\mathbf{K}) c^{+}_{\mathbf{k}\sigma} c_{\mathbf{k}+\mathbf{K}\sigma} + \frac{1}{2} \sum_{\mathbf{q}\neq\mathbf{0}} \sum_{\mathbf{k}\sigma} \sum_{\mathbf{k}'\sigma'} U(\mathbf{q}) c^{+}_{\mathbf{k}+\mathbf{q}\sigma} c^{+}_{\mathbf{k}'-\mathbf{q}\sigma'} c_{\mathbf{k}'\sigma'} c_{\mathbf{k}\sigma}, \qquad (1)$$

where $c_{\mathbf{k}\sigma}$ annihilates an electron specified by momentum $\mathbf{k}$ and spin σ, $\varepsilon_{\mathbf{k}} = \mathbf{k}^2/2m-\mu$ with m the mass of a free electron and μ the chemical potential, $V(\mathbf{K})$ the local electron-ion pseudopotential, and $U(\mathbf{q}) = 4\pi e^2/\mathbf{q}^2$.

Single-electron properties can be analyzed by the study of the thermal Green's function $G_{\mathbf{k},\mathbf{k}+\mathbf{K}}(i\omega_n)$ with ω_n a fermion Matsubara frequency, defined conventionally as

$$G_{\mathbf{k},\mathbf{k}+\mathbf{K}}(i\omega_n) \equiv -\int_0^{1/T} d\tau \langle T_\tau c_{\mathbf{k}\sigma}(\tau) c^{+}_{\mathbf{k}+\mathbf{K}\sigma} \rangle e^{i\omega_n \tau}. \qquad (2)$$

In the correlated-electron approach, we consider 3DEG without V in the first step. Here $G_{\mathbf{k},\mathbf{k}+\mathbf{K}}(i\omega_n)$ is not zero only for $\mathbf{K}=\mathbf{0}$. Thus we simply write $G^{\rm EG}_{\mathbf{k}}(i\omega_n)$ and this function can be determined by the formally exact Dyson equation as shown diagrammatically in Fig. 1(a) with use of the vertex function $\Lambda(\mathbf{k}'i\omega_{n'},\mathbf{k}i\omega_n)$ defined in Fig. 1(c). In the second step, we include V in its lowest order by solving the equation in Fig. 1(b) to obtain $G_{\mathbf{k},\mathbf{k}+\mathbf{K}}(i\omega_n)$ in terms of $G^{\rm EG}_{\mathbf{k}}(i\omega_n)$ and $\Lambda(\mathbf{k}'i\omega_{n'},\mathbf{k}i\omega_n)$.

In order to make the physics as clear as possible, we shall be concerned only with the most interesting case in which $|\mathbf{K}|$ is equal to $2k_{\rm F}$ with $k_{\rm F}$ the Fermi wave number of 3DEG. Then, a band gap Δ opens at the Fermi level with the value of $2V(\mathbf{K})$ in the noninteracting electron gas, while in the interacting system, by expanding the self-energy $\Sigma^{\rm EG}_{\mathbf{k}}(i\omega_n)$ $[=i\omega_n-\varepsilon_{\mathbf{k}}-G^{\rm EG}_{\mathbf{k}}(i\omega_n)^{-1}]$ with respect to ω_n up to first order in line with weak V, we find easily that Δ is given exactly as $2z_{k_{\rm F}}\Lambda(k_{\rm F}0,-k_{\rm F}0)V(\mathbf{K})$ [12] with $G_{-k_{\rm F},k_{\rm F}}(i\omega_n)=z_{k_{\rm F}}\Delta/2[(i\omega_n)^2-(\Delta/2)^2]$ where $z_{k_{\rm F}}$ is the quasi-particle renormalization factor at the Fermi surface. Thus the ratio, $z_{k_{\rm F}}\Lambda(k_{\rm F}0,-k_{\rm F}0)$, quantifies the effect of correlation on the Bragg reflection.

We estimate this ratio quantitatively by employing the local-field correction $G_+(q)$ to represent the effect of the vertex function. Using the values of $G_+(q)$ as supplied by quantum Monte Carlo [13], we can calculate the ratio, together with its components, $z_{k_{\rm F}}$ and $\Lambda(k_{\rm F}0,-k_{\rm F}0)=\{1+\alpha r_s[1-G_+(2k_{\rm F})]/2\pi\}^{-1}$, as a function of r_s the interelectron distance in units of the Bohr radius with $\alpha=(4/9\pi)^{1/3}\approx 0.521$. The results are shown in Fig. 1(d) in which we see that $\Lambda(k_{\rm F}0,-k_{\rm F}0)\approx 1$.

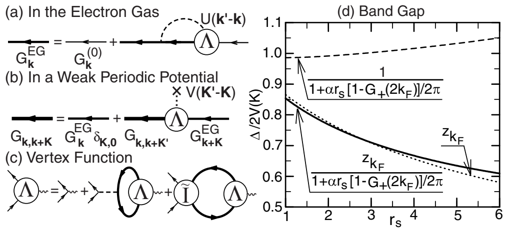

FIG. 1. Diagrammatic representation of $G_{\mathbf{k},\mathbf{k}+\mathbf{K}}(i\omega_n)$ (a) without V and (b) with it in its lowest order. The vertex function $\Lambda(\mathbf{k}'i\omega_{n'},\mathbf{k}i\omega_n)$ is defined in (c) with use of the irreducible electron-hole effective interaction $\widetilde{I}$. In (d), effect of correlation on the Bragg reflection as quantified by $\Delta/2V(\mathbf{K})=z_{k_{\rm F}}/\{1+\alpha r_s[1-G_+(2k_{\rm F})]/2\pi\}$ is shown.

Deviation of the vertex function from unity accounts for the many-body effects on the electron-ion interaction $V_{\rm el-ion}$ and physically this should be small at metallic densities $(1<r_s<6)$ for $q=2k_{\rm F}$ corresponding to the interelectron distance in real space; $V_{\rm el-ion}$ is not modified much from the bare one in the neighborhood of an electron at this distance due to the absence of other electrons by correlation. Thus the ratio is essentially determined only by $z_{k_{\rm F}}$ or the weight of the coherent part, confirming a naively anticipated result that the Bragg reflection occurs only in the coherent part of a quasi-particle.

The importance of $z_{k_{\rm F}}$ in the Bragg reflection prompts us to investigate 1DLL in which $z_{k_{\rm F}}$ vanishes. The Hamiltonian is basically the 1D version of Eq. (1); ε_k is linearized as $\varepsilon_k=v_{\rm F}(k-k_{\rm F})$ $[v_{\rm F}(-k-k_{\rm F})]$ for the right- [left-]moving branch in T and coupling constants, g_1, g_2, and g_4, corresponding to the backward scattering, the forward scattering between the opposite branches, and the forward one within the same branch, respectively, are introduced in U [15]. Using $a_{k\sigma}$ $[b_{k\sigma}]$ the annihilation operator for an electron in the right- [left-]moving branch, we can write V as

$$V=v\sum_{k\sigma}(a^+_{k\sigma}b_{k-2k_{\rm F}\sigma}+b^+_{k-2k_{\rm F}\sigma}a_{k\sigma}), \tag{3}$$

in which only the $K=2k_{\rm F}$ part for $V(K)$ is retained.

The assertion we shall make is that Δ_c due to V corresponding to Δ in the Fermi liquid vanishes in 1DLL. Our strategy to prove it is to find a criterion as to when V turns out to be an irrelevant perturbation. Since the key quantity is $\langle a^+_{k_{\rm F}\sigma}b_{-k_{\rm F}\sigma}\rangle$ or $T\sum_{\omega_n}G_{-k_{\rm F},k_{\rm F}}(i\omega_n)$, we evaluate the expectation value by treating V as a linear perturbation to the system decribed by the Hamiltonian $T+U$. Then, the Kubo's formula provides us

$$\langle a^+_{k_{\rm F}\sigma}b_{-k_{\rm F}\sigma}\rangle=\frac{v}{2}\lim_{\omega\to 0}N(2k_{\rm F},\omega), \tag{4}$$

where $N(q,\omega)$ is the charge-density response function. Thus the problem is reduced to evaluating $N(2k_{\rm F},\omega)$ in the $\omega\to 0$ limit for the system of $T+U$ [14]. The behavior of this function is known well [15] and the result is $N(2k_{\rm F},\omega\to 0)\propto\omega^{\gamma_\rho-1}$ with γ_ρ, given by

$$\gamma_\rho=\sqrt{\frac{1+(g_4+g_1-2g_2)/2\pi v_{\rm F}}{1+(g_4-g_1+2g_2)/2\pi v_{\rm F}}}, \tag{5}$$

for $g_1\geq 0$. This leads us to conclude that $\langle a^+_{k_{\rm F}\sigma}b_{-k_{\rm F}\sigma}\rangle$ vanishes for $g_1>2g_2$ even in the presence of V. More generally, the expectation value is zero in the phases characterized by $N(2k_{\rm F},\omega\to 0)=0$, indicating the irrelevance of V. This irrelevance implies that Δ_c due to V vanishes, because the system is the same as that with $v=0$.

Physically low-lying excitations in 1DLL are rigorously represented by sound waves with wavelengths much longer than $1/2k_{\rm F}$. Thus the effect of V manifests itself after the average of V over a distance longer than its periodicity, which is null and leads to the complete absence of the Bragg reflection. This statement ceases to be valid if V is large enough to destroy the Luttinger-liquid state itself. In this sense, the concept of the Bragg reflection is incompatible with that of Luttinger liquids.

So far no lattice periodicity is considered in $T+U$ and thus the concept of electron filling is irrelevant. Now we include it by treating a 1D system at half-filling on the lattice prescribed by $T+U$ with V possessing periodicity of two lattice units. In site representation, H is given by

$$H = T+V+U = -t\sum_{j\sigma}(c^{+}_{j\sigma}c_{j+1\sigma}+c^{+}_{j+1\sigma}c_{j\sigma}) +v\sum_{j\sigma}(-1)^j c^{+}_{j\sigma}c_{j\sigma} + u\sum_{j} c^{+}_{j\uparrow}c_{j\uparrow}c^{+}_{j\downarrow}c_{j\downarrow}. \quad (6)$$

For the study of competition between V and U in the whole region from $v \gg u$ to $v \ll u$, we implement DMRG to calculate $E(N_\uparrow, N_\downarrow)$ the ground-state energy with N_σ the fixed number of σ-spin electrons in the L-site system under the open-boundary condition. At size L, the charge and spin gaps, $\Delta_c(L)$ and $\Delta_s(L)$, are given as

$$\Delta_c(L) = E(\frac{L}{2}+1, \frac{L}{2}) + E(\frac{L}{2}-1, \frac{L}{2}) - 2E(\frac{L}{2}, \frac{L}{2}), \quad (7)$$

$$\Delta_s(L) = E(\frac{L}{2}+1, \frac{L}{2}-1) - E(\frac{L}{2}, \frac{L}{2}). \quad (8)$$

By using a finite-size scaling as $\Delta_i(L) = (\Delta_i^2 + A_i/L^2 + B_i/L^3 + \cdots)^{1/2}$ for $i = c$ or s [7], we extrapolate the data at $L = 50$, 100, 200, and 400 to obtain the values at $L = \infty$, Δ_c and Δ_s. In Fig. 2, the results thus obtained are plotted as a function of u at $v = 0.5t$. As u increases, both Δ_c and Δ_s decrease from $2v$ (the band gap at $u = 0$) and become very small at around $u = 2.6t$. With the further increase of u, Δ_c increases very rapidly, while Δ_s remains to be zero. In the inset of Fig. 2, the gaps near $u = 2.6t$ are shown in detail. The same overall behavior of the gaps is seen for other values of v of the order of t.

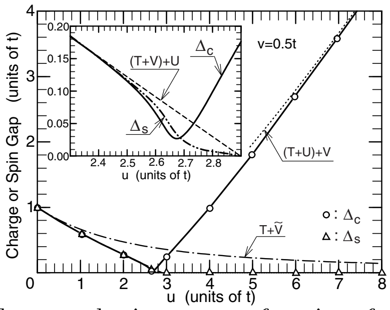

FIG. 2. Charge and spin gaps as a function of u at $v = 0.5t$. Approximate values in the band and correlated-electron approaches are shown by dashed and dotted curves, respectively, while those in HF by the dotted-dashed curve. The inset shows the results around $u = 2.6t$ in a magnified scale.

Let us analyze these results by the comparison with those in both band and correlated-electron approaches. The former approach begins with the Hartree-Fock (HF) approximation which amounts to the one-body problem described by $T+\widetilde{V}$ where we define $\widetilde{V}$ in the same form of V in Eq. (6) by replacing v into $\tilde{v}$, determined through

$$\tilde{v} = v - u\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{dk}{2\pi}\frac{\tilde{v}}{\sqrt{\tilde{v}^2+4t^2\cos^2 k}}\ . \quad (9)$$

In HF we obtain the band insulator (BI) brought about by the full Bragg reflection with $\Delta_c = \Delta_s = 2\tilde{v}$. Since $\tilde{v}$ is always positive, these gaps never vanish, which clearly contradicts the exact results for large u. Even for u as small as t, they do not agree well with the exact ones, as seen by the dotted-dashed curve in Fig. 2.

However, we achieve a surprisingly good improvement by including the correlation effect in second-order perturbation in U with the unperturbed basis in $T+\widetilde{V}$, as shown by the dashed curve in the inset of Fig. 2. In fact, the exact gaps are reproduced quite accurately in this $(T+V)+U$ approach for u from 0 up to about $u_{c0} \equiv 2.45t$. Note that the correlation effect included in this way does not separate Δ_c from Δ_s. Physical mechanism to reduce the gaps from those in HF is the same as explained in 3DEG, namely, the reduction of the the Bragg reflection on the conversion from a free electron to a quasi-particle. Thus we conclude that the state realized in the system for $u < u_{c0}$ is the correlated BI.

For u larger than about $u_{c2} \equiv 2.90t$, on the other hand, Δ_s vanishes, while Δ_c does not, indicating that the state is the MI. The effect of v can be included in Δ_c in the $(T+U)+V$ approach; by examining the exact solution in $T+U$ [16], we can deduce an expansion for Δ_c in u^{-1} up to third order as

$$\Delta_c \approx u - 2\sqrt{v^2+4t^2} + 8\ln 2\ \frac{t^2}{u}\frac{u^2+4v^2}{u^2} - 6\zeta(3)\frac{t^4}{u^3}, \quad (10)$$

with $\zeta(3) \approx 1.202$. The above result is plotted by the dotted curve in Fig. 2 in which we see that the exact result is reproduced quite well for u larger than $5t$.

Now we need to clarify the nature of the state for u at the BI-MI crossover, ranging from u_{c0} to u_{c2}. For that purpose, we calculate D_L a dimensionless localization parameter introduced by Resta and Sorella [5] as

$$D_L = -L\ln\left|\langle\Psi|\exp\left(i\frac{2\pi}{L}\sum_j x_j\right)|\Psi\rangle\right|^2, \quad (11)$$

with Ψ the ground-state wavefunction at $N_\uparrow = N_\downarrow = L/2$ under the open-boundary condition for the L-site system and x_j the position operator at site j. Extrapolation of D_L to the $L \to \infty$ limit gives the value D which is related to λ through $\lambda = \sqrt{D}/2\pi$ in units of the lattice spacing.

The calculated results for both D and D_L at various L's are shown as a function of u in Fig. 3(a). For either $u < u_{c0}$ or $u > u_{c2}$, we see that D_L converges to D at L as small as 100, while for u in-between, even $L = 400$ is not large enough for the convergence. In particular, D seems to diverge for u around $u_{c1} \equiv 2.65t$. Divergence in D, or equivalently that in λ, implies the appearance of a metallic state, indicating the vanishment of Δ_c.

As for $\Delta_c = 0$ at $u = u_{c1}$ and the state for $u_{c1} < u < u_{c2}$, Fabrizio *et al.* [10] have suggested a spontaneously dimerized insulating phase (SDI) by analytical arguments. In fact we find that λ decreases quite rapidly to be less than twice the lattice spacing as u increases from u_{c1}, implying an insulating behavior. Thus we conclude that an insulating phase, most likely SDI, is realized for $u_{c1} < u < u_{c2}$.

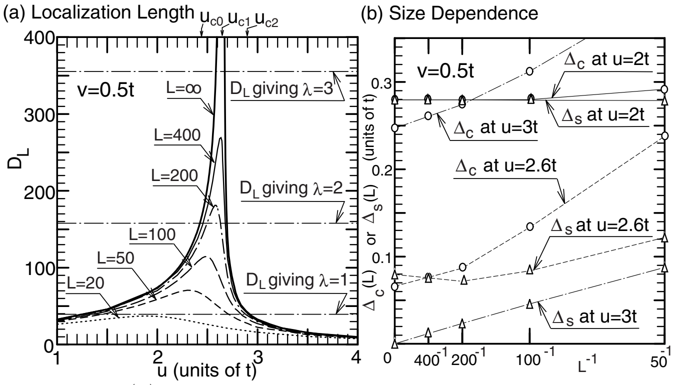

FIG. 3. (a) Dimensionless localization parameter D_L as a function of u at $v=0.5t$ for various system sizes, together with the value extrapolated to $L=\infty$. The values of D_L corresponding to $\lambda = 1$, 2, and 3 are also indicated. (b) Size dependnece of both $\Delta_c(L)$ and $\Delta_s(L)$ at $u = 2t$, $2.6t$, and $3t$.

A remaining problem is that Δ_c never becomes zero in Fig. 2, although we now know that it should be zero at least at $u = u_{c1}$. Thus we reexamine the size dependence of both $\Delta_c(L)$ and $\Delta_s(L)$ carefully and the typical results are plotted in Fig. 3(b). Let us first analyze them in terms of $\Delta_c - \Delta_s$ or the spin-charge separation. Because of one dimensionality, one might assume that $\Delta_c \neq \Delta_s$ should be the case as long as $u \neq 0$, but this is not true; at $u = 2t$ in the BI region, we find that both Δ_c and Δ_s coincide up to at least five digits (which exceeds numerical accuracy) at $L = 200$ or larger. On the other hand, we know that $\Delta_c - \Delta_s = -\Delta_s \neq 0$ at $u = u_{c1}$. Therefore there definitely exists a value of u at which $\Delta_c - \Delta_s$ begins to deviate from zero. We identify u_{c0} as such a value and thus only for u larger than u_{c0} the 1DLL-like spin-charge separation occurs. In this sense, we consider that u_{c0} gives a sharp phase boundary.

In order to find more detailed features of the state at u from u_{c0} to u_{c1}, let us look at Fig. 3 again. As represented at $u = 3t$ in Fig. 3(b), $\Delta_s(L)$ converges to zero very nicely with the increase of L in MI. Similar convergence of both charge and spin gaps is obtained in SDI as well. However, a distinct behavior is seen in the gaps for $u_{c0} < u < u_{c1}$ as illustrated at $u = 2.6t$; both $\Delta_c(L)$ and $\Delta_s(L)$ at $L = 400$ seem to be larger than those extrapolated from the data at smaller L, implying that our data for the gaps are not accurate enough for these u's. This inaccuracy should be due to the large λ which is always longer than the two lattice units for these u's as indicated in Fig. 3(a). This difficulty in obtaining exact values for the gaps in this region can be overcome only by a more accurate calculation of energies at much larger L. Such a calculation is not feasible at present, but we can safely conclude even at the present time that Δ_c is very small, i.e., much smaller than $0.1t$ at most of the values of u in this phase. The nature of small Δ_c and long λ suggests us that a Luttinger-liquid-type quasi-metallic phase appears for $u_{c0} < u < u_{c1}$. Incidentally, each electron in this phase feels V with the spatial average over λ which is longer than the periodicity of V. This implies that the effect of V on the electrons is very small and thus this should be the reason why the feature of BI is lost in the state for $u_{c0} < u < u_{c1}$. Here again we find that the Bragg reflection, a crucial concept to define BI, is incompatible with the Luttinger-liquid feature.

Finally we note that both this phase and SDI deserve special attention, because they are not anticipated in both band and correlated-electron approaches; their existence is entirely due to the competition of V and U.

In conclusion, we have investigated the effect of electron correlation on the Bragg reflection in a variety of situations in various approaches. We have found the incompatibility of the Bragg reflection with the Luttinger liquid, based on which we have suggested a Luttinger-liquid-type quasi-metallic state at the crossover from BI to MI via SDI.

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